

Supporting Information

for

[Fe₄S₄] cubane in sulfite reductases: new insights into bonding properties and reactivity

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Computational Information

Constraints were imposed in the models to best mimic the steric hindrance in the protein environment. The second sphere distal ligands Arg_α98, Arg_α170, Lys_α211, and Lys_α213 were retained in the model due to their positive charge and torsional flexibility. Water molecules present in the crystallographic data are expected to contribute to the reduction of the substrate via coordination with the residues; therefore, two water molecules are included in the active-site model (Figure S1). The distal ligands were truncated at the α-carbon.

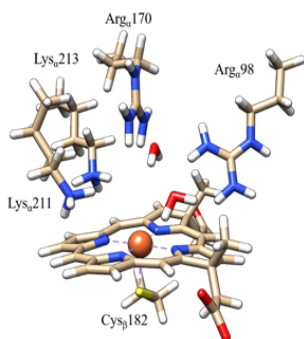


Figure S1. Residue arrangement in constructed model (orange = Fe, brown = C, red = O, blue = N, white = H, yellow = S).

The siroheme, along with two attached carboxylate groups, were included in the model. Experimental studies suggest that the negatively charged carboxylate groups on the siroheme form a tight network with the positively charged residues and are therefore essential components of the active site.¹ Cysteine is the proximal ligand of iron and was truncated at its α-carbon.

Mutational studies suggest that Arg_α98, Arg_α170, Lys_α211, and Lys_α213 are structurally and mechanistically essential to the reactivity of the active site.³ Previous research indicates that the catalytic residues surrounding the active site move in a range of 0.2 - 0.4 Å towards the substrate and effectively provide a caged proton concentration in the active site that stabilizes the negative charge of the substrate and carboxylate groups.² In an attempt to imitate the protein environment accurately, constraints were implemented on the residue ligands proximal to the active site. This approach has been successful in other protein studies.^{3,4} The N-terminus δ-carbon of Lys_α211, Lys_α213, α-carbon of Cys_β182 and N-terminus γ- and δ-carbons of Arg_α98 and Arg_α170 were spatially constrained. Experimental crystallographic studies of substrate-bound structures show that the active site does not undergo significant conformational changes upon substrate binding.¹

The predicted acidities of the side chains determined the active-site protonation scheme. The relative acidities of each residue were estimated using the PROPKA program.^{5,6} The well-suited proton donors, arginine, and lysine, have a typical p*K*_a ~12.50 and ~ 10.50, respectively. In the protein environment, Lys_α213 and Lys_α211 are predicted to have a p*K*_a ~ 6.59 and 9.67, respectively. Lysine has a p*K*_a value close to physiological pH, making the chain a suitable proton donor. Additionally, Arg_α170 and Arg_α98 are predicted to have a p*K*_a of ~11.33 and ~12.97 in the protein. Therefore, all four side-chain residues were protonated in this study. Sirohemes have been experimentally observed to activate various substrates.¹ For this reason, this study includes three substrates (HSO₃⁻, SO₃²⁻, and NO₂⁻). HSO₃⁻ was identified from crystallographic data since one sulfur-oxygen bond was 0.2 Å longer than the others.²

Table S1. Geometric parameters (distances (d) in Å) of the heme species with ligands (without the cubane cluster) optimized at BP86/TZ2P level of theory, together with ligand interaction energies (E_{int}) of the species at B3LYP//BP86/TZ2P, and TPSSh//BP86/TZ2P (kcal/mol)

Species	Spin State, S	d _{Fe-S/N}	Average d _{S-O/N-O}	d _{S-OH}	E _{int} (B3LYP//BP86)	E _{int} (TPSSh//BP86)
HSO ₃ ⁻	0		1.506	1.774		
Heme-Fe ²⁺ -HSO ₃ ⁻	0	2.176	1.530	1.659	-44.5	-42.3
Heme-Fe ²⁺ -HSO ₃ ⁻	1	2.211	1.526	1.659	-41.1	-42.2

Heme-Fe ²⁺ -HSO ₃ ⁻	2	3.233	1.531	1.664	-45.4	-40.6
Heme-Fe ³⁺ -HSO ₃ ⁻	1/2	2.252	1.519	1.656	-37.1	-37.7
Heme-Fe ³⁺ -HSO ₃ ⁻	3/2	2.401	1.514	1.634	-53.9	-52.0
Heme-Fe ³⁺ -HSO ₃ ⁻	5/2	3.448	1.541	1.635	-80.5	-72.0
SO ₃ ²⁻	0		1.558			
Heme-Fe ²⁺ -SO ₃ ²⁻	0	2.277	1.544		-103.8	-102.2
Heme-Fe ²⁺ -SO ₃ ²⁻	1	2.315	1.542		-110.2	-107.6
Heme-Fe ²⁺ -SO ₃ ²⁻	2	3.475	1.563		-112.0	-105.2
Heme-Fe ³⁺ -SO ₃ ²⁻	1/2	2.317	1.538		-148.9	-146.4
Heme-Fe ³⁺ -SO ₃ ²⁻	3/2	2.390	1.533		-151.2	-146.2
Heme-Fe ³⁺ -SO ₃ ²⁻	5/2	3.167	1.557		-126.9	-106.0
NO ₂ ⁻	0		1.277			
Heme-Fe ²⁺ -NO ₂ ⁻	0	1.824	1.328		-56.9	-56.7
Heme-Fe ²⁺ -NO ₂ ⁻	1	1.840	1.326		-51.9	-51.8
Heme-Fe ²⁺ -NO ₂ ⁻	2	2.027	1.356		-48.1	-50.8
Heme-Fe ³⁺ -NO ₂ ⁻	1/2	1.860	1.315		-76.5	-77.4
Heme-Fe ³⁺ -NO ₂ ⁻	3/2	1.918	1.301		-67.6	-69.8
Heme-Fe ³⁺ -NO ₂ ⁻	5/2	2.052	1.341		-48.1	-54.4

Table S2. Results of the EDA analysis (all in kcal/mol) for the low and intermediate-spin siroheme-compounds. E_{Pauli} is the Pauli repulsion, E_{el} is the electrostatic interaction, E_{orb} is the orbital interaction, ΔE_{solv} is the difference in solvation energy between the molecule and the fragments, E_{total} is the total bonding energy at the optimized geometry of the cluster, $E_{\text{total-rel}}$ is the bonding energy in which the relaxation of the individual components has been taken into consideration.

$${}^{\text{a}}E_{\text{steric}} = E_{\text{Pauli}} + E_{\text{el}}$$

Species	E_{Pauli}	E_{el}	$E_{\text{steric}}^{\text{a}}$	E_{orb}	ΔE_{solv}	E_{total}	$E_{\text{total-rel}}$
<i>Intermediate spin (S = 1 (Fe²⁺)/S = 1.5 (Fe³⁺))</i>							
Siro-Fe ²⁺ -HSO ₃ ⁻	236.3	-315.7	-79.4	-113.3	121.0	-71.6	-45.6
Siro-Fe ³⁺ -HSO ₃ ⁻	187.3	-677.6	-490.3	-111.9	419.0	-183.2	-83.7
Siro-Fe ²⁺ -SO ₃ ²⁻	321.1	-511.0	-189.9	-189.3	249.5	-129.7	-104.2
Siro-Fe ³⁺ -SO ₃ ²⁻	188.0	-563.9	-375.8	-123.6	340.1	-159.3	-144.8
Siro-Fe ²⁺ -NO ₂ ⁻	321.7	-322.2	-0.5	-205.9	109.8	-96.6	-42.5
Siro-Fe ³⁺ -NO ₂ ⁻	77.9	-273.4	-195.5	-42.4	160.4	-77.6	-53.6

Low spin (S = 0 (Fe²⁺)/S = 0.5 (Fe³⁺))

Siro-Fe ²⁺ -HSO ₃ ⁻	261.3	-337.6	-76.3	-128.4	126.1	-78.6	-54.3
Siro-Fe ³⁺ -HSO ₃ ⁻	248.5	-718.3	-469.7	-134.6	412.7	-191.6	-91.7
Siro-Fe ²⁺ -SO ₃ ²⁻	297.3	-528.5	-231.2	-172.6	257.5	-146.4	-120.7
Siro-Fe ³⁺ -SO ₃ ²⁻	245.6	-604.7	-359.1	-140.5	333.6	-165.9	-133.8
Siro-Fe ²⁺ -NO ₂ ⁻	141.7	-250.3	-108.7	-101.8	130.6	-79.8	-36.6
Siro-Fe ³⁺ -NO ₂ ⁻	75.8	-270.1	-194.3	-42.6	159.3	-77.7	-56.9

Table S3. Relative energies of the heme and siroheme species with ligands at BP86/TZ2P, B3LYP//BP86/TZ2P, and TPSSH//BP86/TZ2P (kcal/mol)

Species	Spin state, S	Relative Energy (ΔE) BP86	Relative Energy (ΔE) B3LYP//BP86	Relative Energy (ΔE) TPSSH//BP86
Substrate- HSO_3^-				
Siroheme-Fe ²⁺	0	0.0	0.0	0.0
Siroheme-Fe ²⁺	1	19.7	15.9	16.5
Siroheme-Fe ²⁺	2	26.8	1.1	16.0
Siroheme-Fe ³⁺	1/2	0.0	0.0	0.0
Siroheme-Fe ³⁺	3/2	16.0	5.5	13.5
Siroheme-Fe ³⁺	5/2	44.7	26.6	38.2
heme-Fe ²⁺	0	0.9	2.7	3.3
heme-Fe ²⁺	1	0.0	0.0	0.0
heme-Fe ²⁺	2	6.8	-7.5	2.2
heme-Fe ³⁺	1/2	0.0	0.0	0.0
heme-Fe ³⁺	3/2	5.9	1.4	2.8
heme-Fe ³⁺	5/2	8.7	-13.4	0.5
Substrate- SO_3^{2-}				
Siroheme-Fe ²⁺	0	0.0	0.0	0.0
Siroheme-Fe ²⁺	1	18.2	14.0	14.9
Siroheme-Fe ²⁺	2	21.8	0.0	11.2
Siroheme-Fe ³⁺	1/2	0.0	0.0	0.0
Siroheme-Fe ³⁺	3/2	12.2	0.8	8.9
Siroheme-Fe ³⁺	5/2	23.1	2.2	14.7
heme-Fe ²⁺	0	0.7	3.1	3.2
heme-Fe ²⁺	1	0.0	0.0	0.0
heme-Fe ²⁺	2	4.3	-8.9	0.0
heme-Fe ³⁺	1/2	0.0	0.0	0.0
heme-Fe ³⁺	3/2	5.2	0.3	1.8
heme-Fe ³⁺	5/2	18.5	-5.2	19.0
Substrate- NO_2^-				
Siroheme-Fe ²⁺	0	1.8	9.8	7.2
Siroheme-Fe ²⁺	1	0.0	0.0	0.0
Siroheme-Fe ²⁺	2	20.9	15.2	16.4
Siroheme-Fe ³⁺	1/2	0.0	0.0	0.0
Siroheme-Fe ³⁺	3/2	9.9	1.4	6.0
Siroheme-Fe ³⁺	5/2	16.8	-3.2	6.4
heme-Fe ²⁺	0	1.1	5.8	4.5
heme-Fe ²⁺	1	0.0	0.0	0.0
heme-Fe ²⁺	2	8.1	3.3	4.9
heme-Fe ³⁺	1/2	0.0	0.0	0.0
heme-Fe ³⁺	3/2	6.6	9.3	7.4
heme-Fe ³⁺	5/2	24.1	26.5	25.0

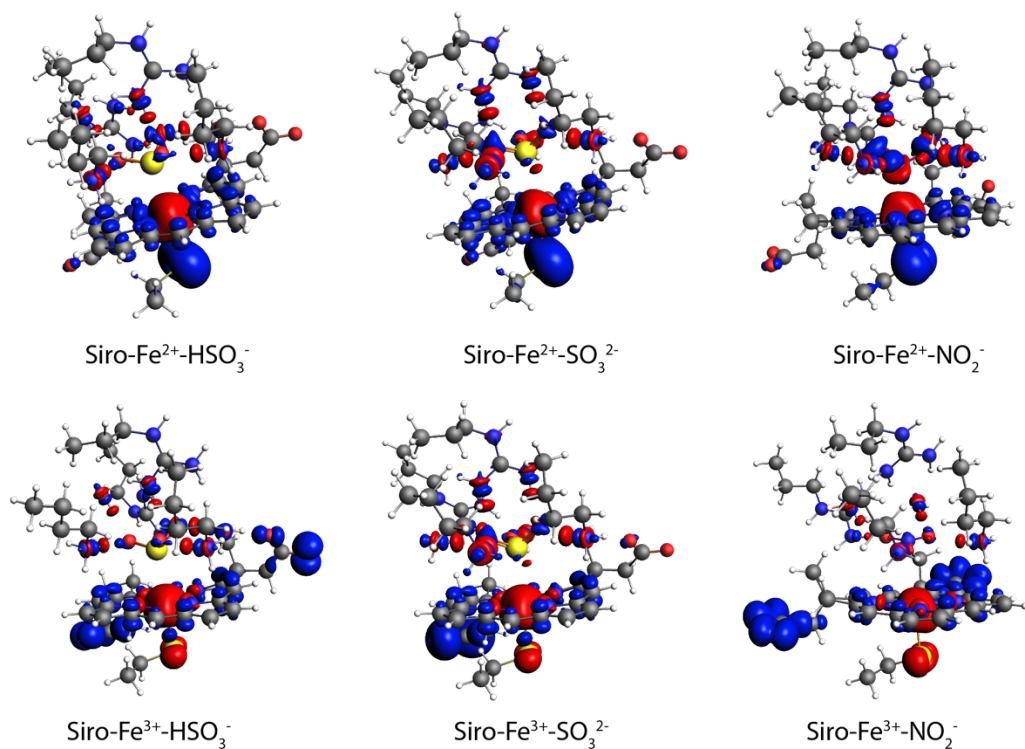


Figure S2. Density difference plots upon complexation of the ligand for the Siro-Fe compounds.

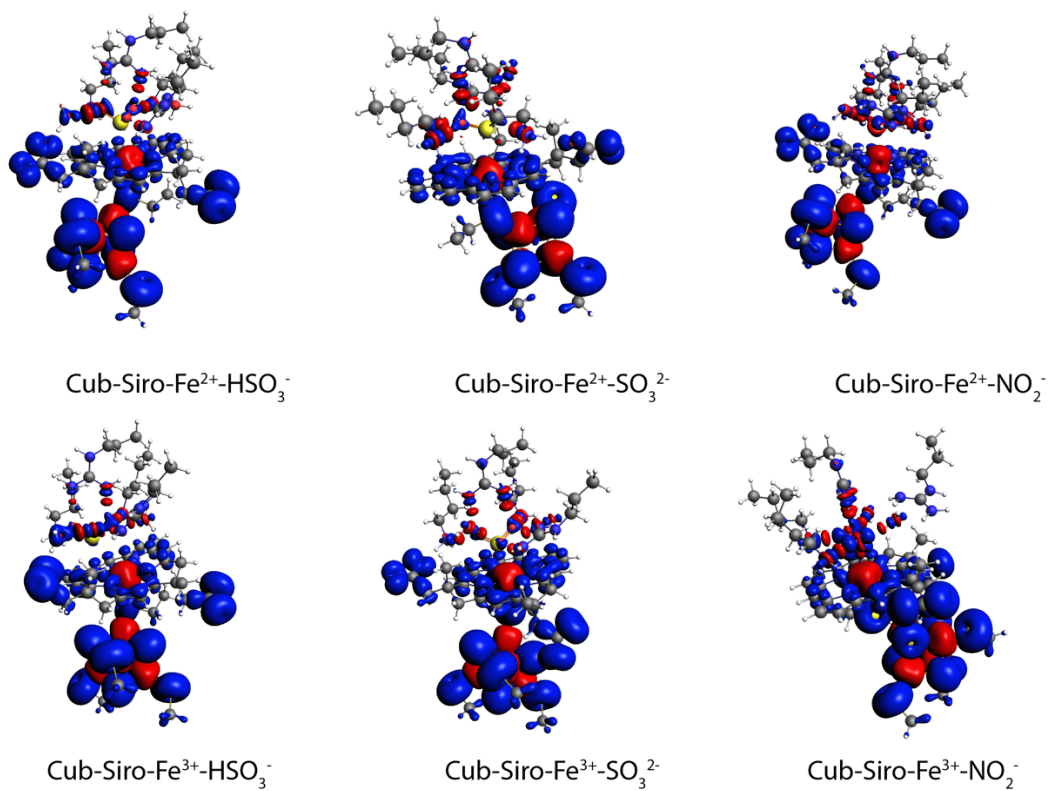


Figure S3. Density difference plots upon complexation of the ligand for the Cub-Siro-Fe compounds.

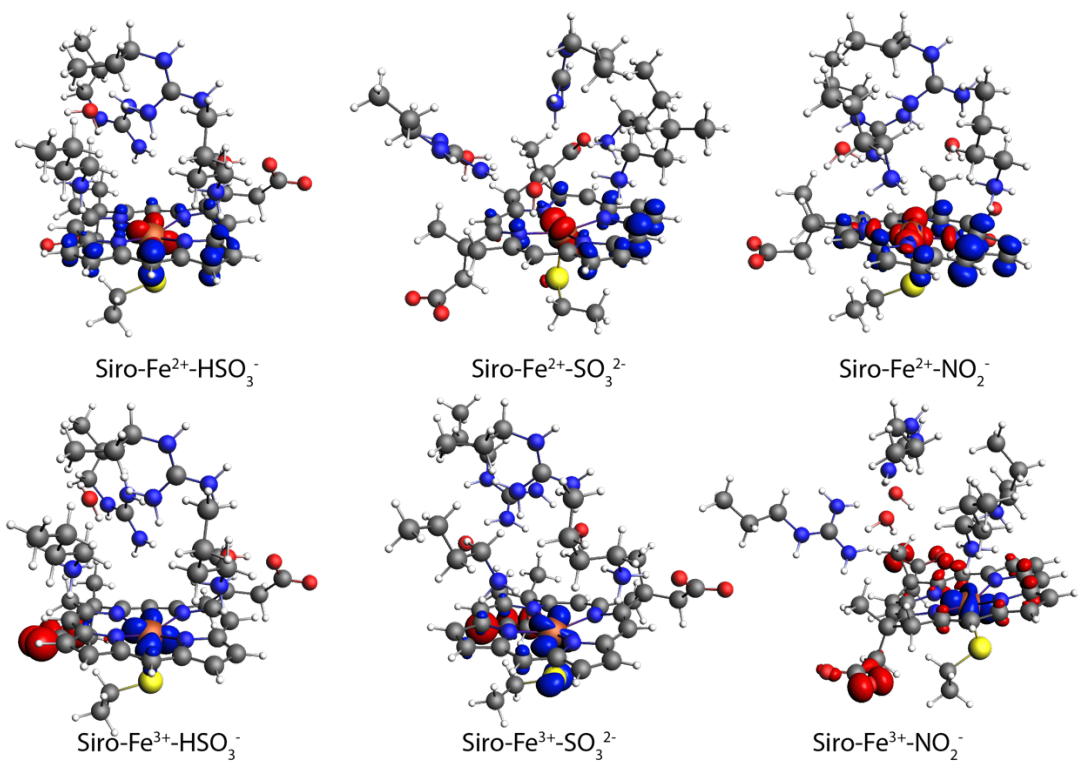


Figure S4. Plots of the dual descriptor for the Siro-Fe compounds.

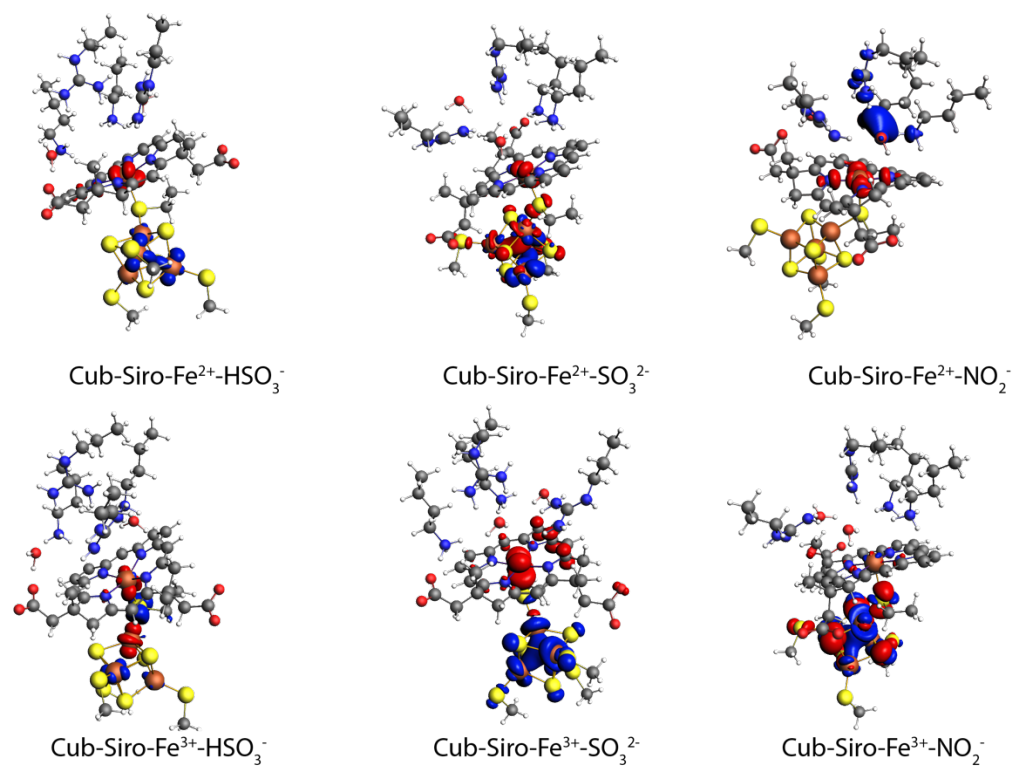


Figure S5. Plots of the dual descriptor for the Cub-Siro-Fe compounds.

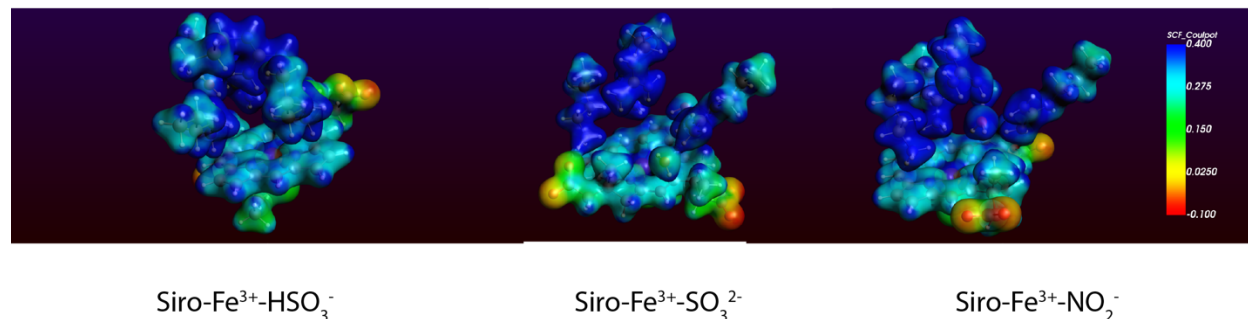
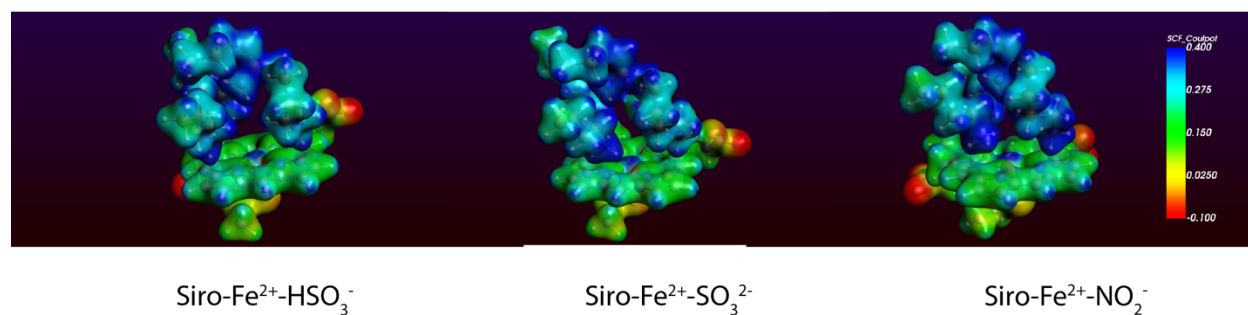


Figure S6. Plots of the electrostatic potential (plotted at the density for isovalue 0.03) for the Siro-Fe compounds.

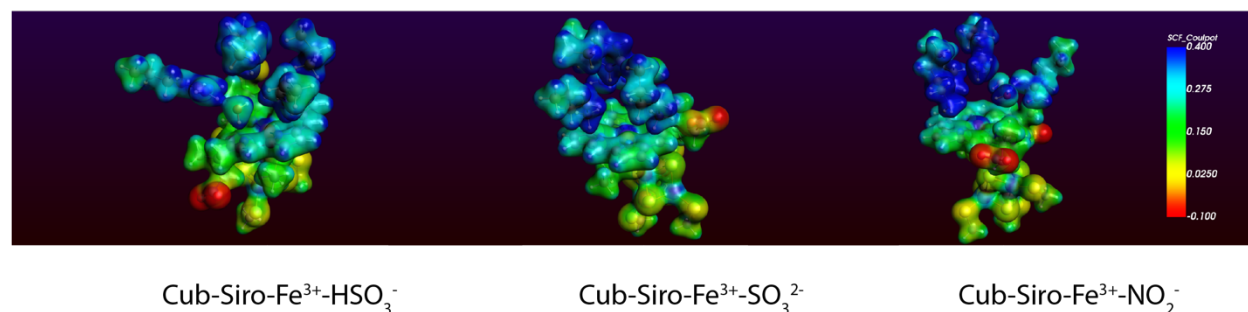
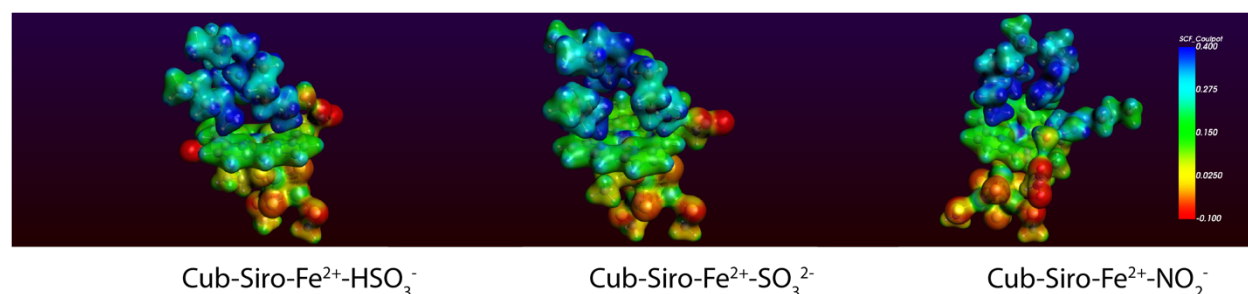


Figure S7. Plots of the electrostatic potential (plotted at the density for isovalue 0.03) for the Cub-Siro-Fe compounds.

Table S4. The cDFT descriptors for the Siro-Fe^{2+/3+}-(HSO₃⁻, SO₃²⁻, NO₂⁻) pre-complexes with and without cubane.

	Siro-Fe ²⁺ -(HSO ₃ ⁻)	Cub-Siro-Fe ²⁺ -(HSO ₃ ⁻)	Siro-Fe ²⁺ -(SO ₃ ²⁻)	Cub-Siro-Fe ²⁺ -(SO ₃ ²⁻)	Siro-Fe ²⁺ -(NO ₂ ⁻)	Cub-Siro-Fe ²⁺ -(NO ₂ ⁻)	Siro-Fe ³⁺ -(HSO ₃ ⁻)	Cub-Siro-Fe ³⁺ -(HSO ₃ ⁻)	Siro-Fe ³⁺ -(SO ₃ ²⁻)	Cub-Siro-Fe ³⁺ -(SO ₃ ²⁻)	Siro-Fe ³⁺ -(NO ₂ ⁻)	Cub-Siro-Fe ³⁺ -(NO ₂ ⁻)
Hardness	0.039	0.034	0.042	0.044	0.033	0.004	0.057	0.026	0.053	0.026	0.053	0.027
Softness	25.920	29.352	23.792	22.681	30.240	247.732	17.588	38.826	18.769	38.799	18.988	36.585
Electrophilicity index	0.251	0.287	0.236	0.216	0.292	2.719	0.354	0.613	0.380	0.630	0.395	0.597
f ⁺ (Fe)	0.138	0.002	0.116	0.003	0.063	0.510	0.682	0.309	0.556	0.057	0.764	0.029
f ⁻ (Fe)	0.693	0.656	0.656	0.160	0.558	0.020	0.002	0.351	0.002	0.631	0.020	0.021
f ⁰ (Fe)	0.416	0.329	0.386	0.082	0.310	0.265	0.342	0.330	0.279	0.344	0.392	0.025
f ⁽²⁾ (Fe)	-0.555	-0.654	-0.540	-0.157	-0.494	0.490	0.681	-0.043	0.554	-0.575	0.744	0.009
Mul. pop (Fe)	0.741	0.765	0.746	0.754	0.577	0.622	0.806	0.785	0.811	0.764	0.793	0.773
Spin mul (Fe)	3.723	3.778	3.741	3.779	3.538	2.659	4.023	3.957	4.023	3.821	4.027	3.808

Table S5. The cDFT descriptors for the Siro-Fe^{2+/3+}-(HSO₃⁻, SO₃²⁻, NO₂⁻) complexes with and without cubane.

	Siro-Fe ²⁺ -HSO ₃ ⁻	Cub-Siro-Fe ²⁺ -HSO ₃ ⁻	Siro-Fe ²⁺ -SO ₃ ²⁻	Cub-Siro-Fe ²⁺ -SO ₃ ²⁻	Siro-Fe ²⁺ -NO ₂ ⁻	Cub-Siro-Fe ²⁺ -NO ₂ ⁻	Siro-Fe ³⁺ -HSO ₃ ⁻	Cub-Siro-Fe ³⁺ -HSO ₃ ⁻	Siro-Fe ³⁺ -SO ₃ ²⁻	Cub-Siro-Fe ³⁺ -SO ₃ ²⁻	Siro-Fe ³⁺ -NO ₂ ⁻	Cub-Siro-Fe ³⁺ -NO ₂ ⁻
Hardness	0.039	0.025	0.042	0.027	0.050	0.033	0.059	0.027	0.057	0.022	0.053	0.028
Softness	25.623	40.376	23.746	36.423	20.155	30.265	17.014	37.555	17.691	45.208	18.925	35.297
Electrophilicity index	0.174	0.301	0.100	0.195	0.197	0.283	0.276	0.487	0.212	0.467	0.311	0.527
f ⁺ (Fe)	0.143	0.004	0.121	0.005	0.337	0.467	0.691	0.444	0.623	0.355	0.764	0.640
f ⁻ (Fe)	0.681	0.690	0.661	0.668	0.105	0.019	0.006	0.220	0.028	0.338	0.002	0.007
f ⁰ (Fe)	0.412	0.347	0.391	0.336	0.221	0.243	0.348	0.332	0.325	0.347	0.383	0.324
f ⁽²⁾ (Fe)	-0.538	-0.686	-0.541	-0.663	0.232	0.448	0.685	0.224	0.595	0.017	0.762	0.633
Mul. pop. (Fe)	0.643	0.701	0.710	0.703	0.689	0.766	0.697	0.803	0.712	0.672	0.789	0.891
Spin pop (Fe)	3.721	3.780	3.759	3.793	3.143	2.685	4.032	4.023	4.054	3.993	4.040	4.142

Table S6. Cartesian coordinates (Å) of the siroheme species (Fe²⁺ & Fe³⁺) with ligands (and without the cubane cluster) optimized at DFT (BP86 functional) using TZ2P basis sets. S is the spin state of the species.

Siroheme (Fe ²⁺) with HSO ₃ ⁻												
S=0			S=1			S=2						
C	50.428910	4.480310	71.588390	C	50.428910	4.480310	71.588390	C	50.428910	4.480310	71.588390	
C	51.175271	5.729258	71.116538	C	51.096387	5.768813	71.106263	C	51.281519	5.659546	71.116010	
C	50.587933	6.288025	69.817141	C	50.454221	6.292275	69.818135	C	50.771782	6.234574	69.790749	
N	51.254217	7.509463	69.361399	N	51.062705	7.529239	69.326368	N	51.516079	7.413905	69.346079	
C	52.419768	7.552660	68.702340	C	52.224009	7.601229	68.662750	C	52.699753	7.396257	68.721819	
N	52.947428	6.441802	68.147537	N	52.814265	6.493056	68.173088	N	53.201990	6.249865	68.217007	
N	53.105165	8.690604	68.603277	N	52.837641	8.770428	68.494331	N	53.432217	8.505448	68.613359	
C	52.322910	2.353310	63.305390	C	52.322910	2.353310	63.305390	C	52.322910	2.353310	63.305390	
C	53.829885	2.456438	63.548808	C	53.840914	2.430532	63.476079	C	53.834217	2.259685	63.523883	
C	54.143630	2.519316	65.053903	C	54.225183	2.464097	64.964903	C	54.182088	2.285077	65.025168	
N	55.454449	3.092325	65.367816	N	55.551213	3.025281	65.227236	N	55.500344	2.853391	65.321526	
C	55.716309	4.401092	65.227732	C	55.810976	4.337586	65.117154	C	55.758700	4.157184	65.160937	
N	54.751357	5.221915	64.831113	N	54.829190	5.169171	64.778427	N	54.790540	4.972179	64.759913	
N	56.959315	4.881410	65.426910	N	57.056161	4.816514	65.287170	N	57.006232	4.643393	65.333103	
C	57.721910	3.753310	61.692390	C	57.721910	3.753310	61.692390	C	57.721910	3.753310	61.692390	
C	57.681910	4.934310	60.688390	C	57.681910	4.934310	60.688390	C	57.681910	4.934310	60.688390	
C	57.222491	6.247312	61.342927	C	56.959725	6.176945	61.211294	C	57.255049	6.255030	61.345635	
C	58.114124	6.614529	62.518793	C	57.784917	6.953865	62.227195	C	58.175004	6.633589	62.497924	
N	57.680793	7.864801	63.206088	N	57.126982	8.250530	62.539890	N	57.717332	7.864253	63.203102	
C	51.935910	3.947310	59.008390	C	51.935910	3.947310	59.008390	C	51.935910	3.947310	59.008390	

C	52.628910	4.440310	60.285390	C	52.628910	4.440310	60.285390	C	52.628910	4.440310	60.285390
C	52.074480	5.784331	60.766786	C	52.116942	5.820953	60.709784	C	52.025031	5.739649	60.829486
C	52.727841	6.242648	62.061156	C	52.735591	6.299503	62.013088	C	52.718937	6.186699	62.107445
N	52.113569	7.505330	62.571100	N	52.140574	7.597282	62.455252	N	52.077645	7.401354	62.700288
Fe	54.427678	10.745899	64.984905	Fe	54.327866	10.914184	65.019259	Fe	54.454916	11.248431	65.012367
C	57.733478	10.610171	65.738228	C	57.593482	10.451721	65.898875	C	57.830191	10.813527	65.671603
C	53.783818	11.837319	68.110722	C	53.646013	11.929605	68.141061	C	53.918789	11.752752	68.303279
C	51.084962	10.554200	64.336571	C	51.007570	10.599316	64.325877	C	51.109122	10.585333	64.545680
C	55.133452	10.561906	61.636719	C	55.140101	10.832044	61.705005	C	55.064808	10.466048	61.658031
N	55.506656	10.965503	66.635694	N	55.360747	10.972840	66.712673	N	55.655773	11.110083	66.708668
C	56.849410	10.646135	66.781415	C	56.676992	10.516594	66.898302	C	57.007499	10.835040	66.772782
C	57.206239	10.563690	68.265584	C	56.952986	10.380688	68.393004	C	57.427180	10.701022	68.240592
C	56.702529	9.277015	68.961722	C	56.326537	9.132032	69.057796	C	56.998619	9.358607	68.883546
C	58.684557	10.779749	68.577234	C	58.429860	10.472002	68.766921	C	58.906732	10.958900	68.508880
C	59.712387	9.661015	68.256696	C	59.362870	9.267038	68.493335	C	59.960763	9.889363	68.105626
O	59.353109	8.548578	67.717227	O	58.953978	8.222626	67.852590	O	59.623269	8.789144	67.528062
O	60.894649	9.923955	68.574964	O	60.524319	9.375619	68.941259	O	61.142910	10.180530	68.398941
C	56.261778	11.698059	68.744334	C	56.091620	11.588252	68.859337	C	56.444223	11.758815	68.823955
C	55.093048	11.512973	67.804723	C	54.946970	11.526654	67.872433	C	55.243057	11.550571	67.924372
N	52.757094	11.004997	66.061204	N	52.647885	11.094231	66.076611	N	52.774593	11.030938	66.271970
C	52.693471	11.538217	67.309418	C	52.566636	11.641245	67.311701	C	52.775253	11.472189	67.545804
C	51.256560	11.825071	67.737309	C	51.118027	11.917884	67.710707	C	51.352307	11.716137	68.047221
C	50.949993	11.550760	69.208813	C	50.791970	11.678871	69.184109	C	51.102970	11.309172	69.497879
C	50.976577	13.319968	67.402765	C	50.824229	13.399260	67.333169	C	51.080524	13.238138	67.856629
C	49.515667	13.722040	67.710091	C	49.362662	13.801960	67.636220	C	49.643841	13.622981	68.282269
O	49.309939	14.361085	68.783185	O	49.162023	14.487890	68.680777	O	49.509793	14.148629	69.425499
O	48.636608	13.353764	66.871508	O	48.479529	13.389179	66.823436	O	48.714727	13.351986	67.462111
C	50.496094	10.897594	66.772574	C	50.382667	10.954058	66.758344	C	50.542335	10.886744	67.024275
C	51.460145	10.773806	65.629133	C	51.348605	10.835047	65.616543	C	51.481658	10.806619	65.847958
N	53.325477	10.555033	63.312373	N	53.280564	10.636897	63.332108	N	53.312829	10.575628	63.391839
C	51.958612	10.512387	63.232699	C	51.900280	10.560846	63.223102	C	51.941108	10.503746	63.396745
C	51.545824	10.397419	61.861249	C	51.531810	10.451654	61.862447	C	51.469639	10.301962	62.055494
C	52.695350	10.356011	61.096716	C	52.718282	10.445632	61.114479	C	52.584889	10.217160	61.234158
C	53.800084	10.469747	62.006762	C	53.795260	10.606331	62.040270	C	53.735307	10.400985	62.077389
N	56.103866	10.666073	63.895381	N	56.049414	10.741246	63.991323	N	56.149042	10.721296	63.857477
C	56.202243	10.700127	62.510009	C	56.185944	10.981895	62.628064	C	56.186195	10.665701	62.474709
C	57.579502	10.836754	62.123589	C	57.566776	11.178739	62.323865	C	57.546518	10.807857	62.036243
C	58.317391	10.873192	63.291091	C	58.280804	10.962904	63.508887	C	58.326643	10.943131	63.177724
C	57.383981	10.749304	64.374092	C	57.321403	10.712581	64.526792	C	57.436335	10.875630	64.299242
S	54.319962	8.617640	65.102340	S	54.189106	8.573009	65.119953	S	54.452217	8.342708	65.136656
O	55.103118	7.813192	64.064044	O	54.969696	7.822746	64.053222	O	55.114717	7.593265	63.986453
O	52.923503	8.018019	65.130658	O	52.781866	8.025854	65.120824	O	53.047192	7.790698	65.279007
O	54.888233	7.889942	66.551317	O	54.757670	7.913392	66.517152	O	55.164838	7.589191	66.505287
C	52.934910	13.851310	62.600390	C	52.934910	13.851310	62.600390	C	52.934910	13.851310	62.600390
C	52.981630	13.681093	64.114347	C	52.924673	13.714589	64.120828	C	52.840023	13.935156	64.117895
S	54.576735	13.043577	64.745815	S	54.492497	13.055879	64.785251	S	54.429142	13.556287	64.964786
H	54.952579	6.213257	64.590072	H	55.014020	6.164737	64.573644	H	54.994845	5.955825	64.504525
H	50.859949	4.098561	72.521787	H	50.894426	4.123396	72.515136	H	50.805035	4.084113	72.539366
H	50.483889	3.677547	70.839955	H	50.518292	3.681644	70.838649	H	50.440189	3.661159	70.855580
H	49.367815	4.697171	71.771864	H	49.359740	4.636387	71.787745	H	49.383547	4.782682	71.739612
H	51.127511	6.511794	71.887259	H	51.020106	6.548382	71.877732	H	51.270967	6.459331	71.870508
H	52.239281	5.501338	70.959377	H	52.168330	5.598993	70.929980	H	52.329582	5.349486	70.994531
H	50.625218	5.535635	69.017926	H	50.492799	5.531095	69.026213	H	50.793945	5.472260	68.999933
H	49.529216	6.540835	69.950098	H	49.391628	6.509846	69.977607	H	49.724754	6.546230	69.885141
H	53.730810	6.623947	67.511569	H	53.589749	6.667224	67.527814	H	53.998033	6.379643	67.586677
H	52.309738	5.717158	67.830554	H	52.230682	5.696542	67.940771	H	52.546163	5.531726	67.922162
H	53.849574	8.739610	67.901240	H	53.607579	8.826347	67.826588	H	54.188019	8.502523	67.923959
H	52.779941	9.558520	69.014460	H	52.491662	9.636522	68.892399	H	53.113222	9.407327	68.954736

H	52.098515	2.145828	62.253601	H	52.043391	2.161861	62.263641	H	52.056904	2.182954	62.256917
H	51.811411	3.281528	63.594058	H	51.843152	3.286552	63.628543	H	51.939300	3.336357	63.608796
H	54.224918	3.355434	63.055177	H	54.225092	3.332419	62.979624	H	54.332259	3.098531	63.019340
H	54.357109	1.600713	63.106088	H	54.333207	1.574693	62.995090	H	54.236033	1.342647	63.074023
H	54.125205	1.516032	65.490802	H	54.219643	1.453466	65.385503	H	54.173940	1.274131	65.443115
H	53.365633	3.095872	65.578181	H	53.476225	3.036157	65.534682	H	53.419251	2.852818	65.580187
H	53.768053	4.958284	64.910122	H	53.846511	4.907509	64.879822	H	53.806763	4.728425	64.894875
H	57.686187	4.248044	65.738156	H	57.790465	4.172664	65.557845	H	57.740536	4.022036	65.651506
H	57.093695	5.873804	65.658460	H	57.178545	5.804090	65.578521	H	57.116073	5.624624	65.582945
H	57.909314	2.806955	61.170059	H	58.233921	2.887594	61.255061	H	57.894053	2.805004	61.168328
H	56.762329	3.660422	62.221591	H	56.702439	3.445153	61.964050	H	56.767202	3.670699	62.231976
H	58.512752	3.877002	62.441854	H	58.247153	4.025292	62.617265	H	58.521489	3.869584	62.433626
H	58.677304	5.073553	60.241790	H	58.706012	5.206399	60.392121	H	58.670970	5.055416	60.222522
H	56.996514	4.694570	59.864689	H	57.175738	4.597598	59.772931	H	56.978100	4.703218	59.877685
H	56.186430	6.134077	61.701544	H	55.992728	5.891486	61.656696	H	56.227935	6.152881	61.732462
H	57.219300	7.061152	60.603766	H	56.736007	6.846982	60.367091	H	57.236838	7.063187	60.600455
H	59.154583	6.755252	62.204014	H	58.780675	7.175052	61.826375	H	59.202785	6.802463	62.157662
H	58.091926	5.828716	63.280503	H	57.908128	6.409369	63.170223	H	58.193992	5.838969	63.250951
H	57.885217	8.733221	62.671221	H	56.807253	8.734651	61.690452	H	57.931300	8.746338	62.696955
H	58.159860	7.942022	64.116403	H	57.760000	8.935036	63.009093	H	58.135107	7.922057	64.154512
H	52.349548	2.985263	58.680626	H	52.311611	2.960834	58.708258	H	52.392803	3.017105	58.647939
H	52.062422	4.666717	58.187957	H	52.106479	4.641679	58.174490	H	52.009313	4.693679	58.205822
H	50.858020	3.812875	59.174317	H	50.850872	3.863792	59.159957	H	50.869763	3.752227	59.189621
H	53.711318	4.536468	60.107870	H	53.717634	4.484812	60.127933	H	53.700170	4.598486	60.085412
H	52.509308	3.695838	61.081223	H	52.458946	3.726233	61.099678	H	52.571269	3.665913	61.059294
H	50.988080	5.691287	60.926933	H	51.022658	5.774303	60.832158	H	50.952890	5.587139	61.033268
H	52.217226	6.550097	59.989164	H	52.316170	6.555148	59.914314	H	52.096870	6.534305	60.071635
H	53.798412	6.441479	61.940644	H	53.815319	6.462217	61.928622	H	53.771295	6.440479	61.942544
H	52.605069	5.493790	62.852158	H	52.561896	5.580775	62.822863	H	52.672555	5.403505	62.872594
H	52.286032	8.324194	61.949072	H	52.414074	8.412525	61.857019	H	52.202831	8.259154	62.113906
H	52.465951	7.764682	63.539945	H	52.404856	7.836932	63.447688	H	52.460812	7.620403	63.659226
H	58.791321	10.491266	65.961857	H	58.625597	10.219986	66.154280	H	58.900175	10.720589	65.848757
H	53.595369	12.313119	69.071140	H	53.446383	12.401963	69.100125	H	53.757540	12.150926	69.304240
H	50.019473	10.462550	64.130318	H	49.947848	10.477594	64.102296	H	50.039757	10.481374	64.359615
H	55.357336	10.545339	60.570263	H	55.379094	10.939423	60.647254	H	55.246380	10.385162	60.586008
H	57.211823	8.381516	68.604235	H	56.741181	8.197815	68.676738	H	57.537760	8.504725	68.474308
H	55.623206	9.156303	68.835222	H	55.241064	9.121806	68.937163	H	55.922269	9.197571	68.771621
H	56.901351	9.372395	70.038039	H	56.535736	9.177992	70.135609	H	57.213883	9.410923	69.959586
H	59.047985	11.691643	68.081621	H	58.891796	11.343200	68.279287	H	59.219983	11.900533	68.034846
H	58.790348	10.966316	69.656347	H	58.509679	10.658070	69.847904	H	59.049263	11.108140	69.589599
H	51.141590	10.501184	69.476915	H	51.012375	10.646932	69.496851	H	51.350519	10.250592	69.667260
H	49.891469	11.749189	69.415350	H	49.723375	11.848446	69.363584	H	50.046706	11.446292	69.758032
H	51.537819	12.188738	69.879547	H	51.345717	12.357587	69.843626	H	51.694279	11.909136	70.199888
H	51.184423	13.480603	66.336951	H	51.020636	13.527129	66.260664	H	51.237031	13.486944	66.797975
H	51.665142	13.941012	67.989407	H	51.511682	14.044368	67.894448	H	51.806610	13.799427	68.457664
H	50.344783	9.908388	67.239392	H	50.254956	9.971452	67.246827	H	50.354520	9.872957	67.419904
H	50.513059	10.369216	61.524890	H	50.510515	10.387124	61.496535	H	50.424666	10.232937	61.763605
H	52.784680	10.302439	60.015570	H	52.825867	10.435721	60.033339	H	52.610193	10.080533	60.156454
H	57.933000	10.918243	61.099673	H	57.965426	11.381080	61.333385	H	57.875223	10.827317	61.000485
H	59.393097	10.970344	63.406313	H	59.353742	11.026955	63.667418	H	59.404844	11.063516	63.236931
H	55.899075	7.851979	66.530047	H	55.815029	7.800098	66.460060	H	56.174592	7.728140	66.451747
H	53.096872	12.893636	62.094201	H	53.042700	12.877609	62.115818	H	53.254906	12.851964	62.287488
H	52.184516	13.007721	64.448820	H	52.108779	13.061985	64.449347	H	52.081880	13.235637	64.494218
H	52.812045	14.646285	64.612725	H	52.785255	14.693459	64.600457	H	52.539468	14.942833	64.435300
H	50.947329	8.379558	69.786037	H	50.704293	8.400271	69.705537	H	51.228691	8.306966	69.736259
H	56.161382	2.502231	65.790200	H	56.276827	2.422645	65.596955	H	56.207777	2.267906	65.750050
H	56.650409	7.880888	63.444873	H	56.269936	8.147174	63.151184	H	56.680138	7.847956	63.384953
H	51.094666	7.412949	62.636736	H	51.116597	7.560288	62.421946	H	51.065814	7.269524	62.798827

H	51.959207	14.251818	62.281748	H	51.992717	14.306988	62.261376	H	51.958276	14.062610	62.138142
H	53.716295	14.546233	62.263289	H	53.762479	14.493056	62.269701	H	53.662482	14.578330	62.214378
O	51.969607	5.504782	65.447264	O	52.033482	5.425716	65.378798	O	52.067338	5.278243	65.568422
H	52.247174	6.462006	65.422147	H	52.234047	6.400979	65.359527	H	52.346521	6.233833	65.545410
H	51.020991	5.495099	65.236546	H	51.092143	5.345378	65.152098	H	51.115075	5.270743	65.375094
O	57.546089	7.748018	66.127978	O	57.242655	7.538295	66.187195	O	57.756034	7.954927	66.018454
H	57.399262	8.671899	65.798225	H	57.375974	8.270342	65.548068	H	57.534054	8.896037	65.783698
H	58.253485	8.010569	66.857803	H	57.911661	7.870659	66.970870	H	58.501869	8.210748	66.710314
H	51.883750	1.537267	63.896950	H	51.900005	1.537067	63.908443	H	51.791732	1.596540	63.900019
H	55.986740	11.622704	69.802804	H	55.771099	11.520429	69.905480	H	56.228405	11.616257	69.888963
H	56.719690	12.684843	68.564760	H	56.643742	12.532095	68.717063	H	56.838054	12.777527	68.674877
H	49.524004	11.310940	66.482882	H	49.400436	11.338736	66.463727	H	49.580005	11.356439	66.791942

Siroheme (Fe³⁺) with HSO₃⁻

S=1/2			S=3/2			S=5/2					
C	50.428910	4.480310	71.588390	C	50.428910	4.480310	71.588390	C	50.428910	4.480310	71.588390
C	51.154086	5.796995	71.311293	C	51.544341	5.474620	71.258868	C	51.456976	5.573305	71.295666
C	52.099817	5.694385	70.118169	C	51.195917	6.326174	70.034664	C	50.975694	6.499261	70.175184
N	52.798253	6.967238	69.924186	N	52.155944	7.398325	69.781233	N	51.896512	7.592614	69.865579
C	53.680759	7.211890	68.953912	C	53.191524	7.369718	68.936959	C	52.889815	7.530964	68.975552
N	53.930005	6.302026	67.995902	N	53.479051	6.297866	68.182217	N	53.185880	6.369506	68.357845
N	54.387965	8.354167	68.937029	N	54.022004	8.426731	68.852661	N	53.589700	8.619060	68.652023
C	52.322910	2.353310	63.305390	C	52.322910	2.353310	63.305390	C	52.322910	2.353310	63.305390
C	53.831949	2.435747	63.531255	C	53.836802	2.267017	63.492018	C	53.841624	2.320692	63.481325
C	54.155114	2.500671	65.030717	C	54.201315	2.202792	64.985322	C	54.219124	2.225884	64.969236
N	55.518106	2.946650	65.324546	N	55.563042	2.649350	65.279748	N	55.578838	2.683443	65.268184
C	55.921021	4.216851	65.172996	C	55.931582	3.937228	65.187912	C	55.928341	3.972374	65.201742
N	55.036079	5.148727	64.823940	N	55.017779	4.860644	64.909493	N	55.006817	4.897868	64.967946
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C	57.721910	3.753310	61.692390	C	57.721910	3.753310	61.692390	C	57.721910	3.753310	61.692390
C	57.681910	4.934310	60.688390	C	57.681910	4.934310	60.688390	C	57.681910	4.934310	60.688390
C	57.316383	6.270006	61.354828	C	57.300028	6.258937	61.374044	C	57.354770	6.269785	61.375268
C	58.252404	6.605638	62.509298	C	58.207304	6.568971	62.560116	C	58.312320	6.564166	62.522980
N	57.871132	7.875874	63.193288	N	57.769943	7.786294	63.305556	N	57.924210	7.800100	63.267131
C	51.935910	3.947310	59.008390	C	51.935910	3.947310	59.008390	C	51.935910	3.947310	59.008390
C	52.628910	4.440310	60.285390	C	52.628910	4.440310	60.285390	C	52.628910	4.440310	60.285390
C	52.071857	5.766725	60.807944	C	52.016258	5.717946	60.863414	C	51.956556	5.656011	60.932074
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N	52.201325	7.464815	62.637267	N	52.129575	7.372961	62.738195	N	52.054009	7.258491	62.855603
Fe	54.622748	10.846929	64.731832	Fe	54.679599	11.040090	64.782688	Fe	54.693000	11.332214	64.932293
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C	57.686570	11.203463	67.883409	C	57.501422	11.068563	68.203355	C	57.533337	10.792067	68.300600
C	58.204681	9.847546	68.396325	C	57.781344	9.646626	68.725298	C	57.074184	9.466696	68.956430
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C	60.125414	12.196143	67.609030	C	60.070965	11.704760	68.224581	C	60.056525	9.957314	68.233470
O	60.877641	13.319561	67.750324	O	60.965375	12.661265	68.591611	O	59.712098	8.855330	67.663235
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C	56.390798	11.586392	68.624096	C	56.200017	11.613558	68.823944	C	56.542712	11.871985	68.823120
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C	51.472198	11.118884	67.734332	C	51.334721	11.391336	67.566872	C	51.498013	11.839657	67.881270
C	51.297702	10.322996	69.030719	C	51.017564	10.739808	68.913223	C	51.208043	11.400614	69.316392
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O	49.534538	13.010453	69.695844	O	49.288001	13.524897	69.124649	O	49.523584	14.186483	69.158249
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C	50.685490	10.509442	66.563207	C	50.626677	10.692180	66.394797	C	50.710329	11.026712	66.831707
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C	52.842444	10.312162	60.876618	C	53.164257	10.278609	60.869722	C	52.957937	10.187542	61.174040
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H	56.370870	12.654475	68.887128	H	56.268936	12.693936	69.024912	H	56.945982	12.885144	68.661384
H	49.736093	11.030505	66.391692	H	49.697582	11.202285	66.114282	H	49.786379	11.536363	66.532814

Siroheme (Fe²⁺) with SO₃²⁻

S=0			S=1			S=2					
C	51.422358	3.380522	70.997438	C	51.422358	3.380522	70.997438	C	51.422358	3.380522	70.997438
C	51.652695	4.214206	69.734214	C	51.675545	4.200447	69.729184	C	51.737950	4.239196	69.773310
C	52.747055	5.264881	69.920259	C	52.734065	5.285060	69.931909	C	52.770746	5.324263	70.073202
N	52.971919	5.991034	68.672322	N	52.976876	5.993345	68.676440	N	53.072590	6.070434	68.855613
C	54.007741	6.821671	68.438630	C	53.987519	6.856710	68.455157	C	54.176177	6.811912	68.644595
N	54.891866	7.080540	69.413674	N	54.834256	7.169507	69.445175	N	55.059980	7.010621	69.634250
N	54.156949	7.378819	67.238930	N	54.147326	7.400489	67.250069	N	54.390063	7.350995	67.446460
C	55.076348	1.425184	63.280932	C	55.076348	1.425184	63.280932	C	55.076348	1.425184	63.280932
C	56.450302	1.990685	63.631337	C	56.463274	1.963779	63.622201	C	56.536442	1.743374	63.594057
C	56.675846	2.069232	65.151447	C	56.702600	2.016326	65.141154	C	56.829069	1.672407	65.106542

N	57.701753	3.035503	65.536548	N	57.743433	2.962561	65.533880	N	57.905132	2.558955	65.539015
C	57.527384	4.367344	65.384644	C	57.584175	4.298142	65.415363	C	57.780046	3.903786	65.501905
N	56.310360	4.850351	65.136348	N	56.373035	4.800996	65.172071	N	56.578289	4.448245	65.308987
N	58.557883	5.207147	65.502924	N	58.621861	5.124156	65.567995	N	58.841717	4.692801	65.687488
C	60.333112	3.765595	62.506421	C	60.333112	3.765595	62.506421	C	60.333112	3.765595	62.506421
C	60.256756	4.891209	61.442682	C	60.256756	4.891209	61.442682	C	60.256756	4.891209	61.442682
C	59.943389	6.266893	62.037255	C	59.981039	6.269466	62.054243	C	59.997912	6.275061	62.043770
C	61.012349	6.775353	63.003133	C	61.069816	6.736712	63.019977	C	61.138710	6.789146	62.922454
N	60.659405	8.133666	63.483233	N	60.735102	8.078794	63.554606	N	60.754386	8.093374	63.518726
C	55.161658	2.803979	58.893853	C	55.161658	2.803979	58.893853	C	55.161658	2.803979	58.893853
C	55.522484	3.451533	60.237172	C	55.522484	3.451533	60.237172	C	55.522484	3.451533	60.237172
C	55.797815	4.950909	60.176744	C	55.725887	4.963174	60.173370	C	55.732628	4.965166	60.244796
C	56.079177	5.461527	61.579917	C	56.039435	5.492031	61.562532	C	56.079722	5.389186	61.666404
N	56.158892	6.935969	61.678710	N	56.051521	6.968480	61.649268	N	56.104315	6.855570	61.883530
Fe	56.621153	10.468377	64.048043	Fe	56.724968	10.554139	63.908765	Fe	56.632123	10.793307	63.946394
C	60.004459	10.871343	63.958120	C	60.144811	10.824506	63.994460	C	60.066648	10.901871	63.793589
C	56.603704	11.659616	67.192767	C	56.610154	11.750435	67.063090	C	56.779710	11.502290	67.261389
C	53.255208	9.973709	64.155207	C	53.350454	9.970144	63.974004	C	53.320415	9.881507	64.284213
C	56.623800	9.787665	60.654181	C	56.853737	9.725932	60.558493	C	56.559919	9.682254	60.618982
N	58.027208	10.933018	65.365650	N	58.103280	10.968399	65.306864	N	58.177640	11.033997	65.313673
C	59.400944	10.814126	65.172162	C	59.490980	10.802770	65.175929	C	59.528911	10.922814	65.051510
C	60.111383	10.726916	66.511769	C	60.125039	10.734570	66.552546	C	60.304788	10.864883	66.365842
C	59.997798	9.291077	67.075888	C	59.945764	9.323982	67.158453	C	60.271522	9.432741	66.950454
C	61.569165	11.190575	66.510229	C	61.595387	11.154605	66.615110	C	61.741454	11.386272	66.295177
C	62.677092	10.327874	65.842372	C	62.706249	10.203310	66.088167	C	62.849592	10.552707	65.587951
O	62.393802	9.253606	65.201915	O	62.421475	9.178539	65.373857	O	62.577979	9.453720	64.987494
O	63.845338	10.766594	65.994091	O	63.876955	10.530359	66.413285	O	64.003907	11.045401	65.666514
C	59.157809	11.634060	67.324360	C	59.159282	11.697386	67.285580	C	59.346327	11.721732	67.236958
C	57.839248	11.399600	66.620203	C	57.864677	11.469330	66.531754	C	58.005056	11.407606	66.603098
N	55.198498	10.738344	65.424916	N	55.253019	10.777986	65.281152	N	55.270306	10.582755	65.576229
C	55.381020	11.329440	66.636671	C	55.405052	11.389686	66.479904	C	55.519682	11.123625	66.785905
C	54.061291	11.650623	67.328795	C	54.061040	11.685343	67.142629	C	54.227487	11.388601	67.560102
C	54.056327	11.380792	68.834308	C	54.035126	11.457849	68.654253	C	54.280593	10.982589	69.034080
C	53.752680	13.145572	67.023796	C	53.710017	13.160895	66.792343	C	53.940623	12.912021	67.404814
C	52.407295	13.612094	67.620088	C	52.339143	13.597206	67.354172	C	52.612416	13.334596	68.072869
O	52.455490	14.296533	68.685617	O	52.346990	14.304908	68.405092	O	52.691645	13.867998	69.219635
O	51.352715	13.256414	67.007907	O	51.308830	13.195782	66.729852	O	51.543800	13.093956	67.430926
C	53.106105	10.722205	66.562084	C	53.149176	10.703888	66.386176	C	53.212999	10.554329	66.746717
C	53.855827	10.445076	65.289582	C	53.911323	10.444837	65.118042	C	53.929638	10.313092	65.442162
N	55.234933	9.932519	62.689375	N	55.381047	9.924296	62.542599	N	55.218292	9.895958	62.683007
C	53.896830	9.746298	62.921666	C	54.020666	9.740765	62.746526	C	53.906999	9.663455	63.006925
C	53.224399	9.337620	61.723302	C	53.389551	9.349293	61.544611	C	53.197925	9.186921	61.852784
C	54.172988	9.302760	60.722679	C	54.379677	9.313088	60.557192	C	54.100958	9.142503	60.805565
C	55.416940	9.690446	61.328267	C	55.604580	9.692403	61.188113	C	55.361755	9.600404	61.329601
N	58.025899	10.351463	62.599006	N	58.206810	10.313660	62.544719	N	58.053306	10.356304	62.462449
C	57.837727	10.107955	61.241470	C	58.061036	10.050619	61.188084	C	57.813118	10.039316	61.136206
C	59.070324	10.280786	60.526225	C	59.319924	10.186232	60.529568	C	59.036272	10.142934	60.394197
C	60.011131	10.667413	61.455488	C	60.242951	10.576030	61.500476	C	60.015786	10.543279	61.287366
C	59.341601	10.707800	62.727321	C	59.536591	10.658519	62.728084	C	59.381266	10.672894	62.570711
S	56.859650	8.377520	64.809984	S	56.933166	8.326857	64.859445	S	57.243820	7.969910	65.148064
O	58.202012	7.699300	64.491433	O	58.285752	7.654379	64.624914	O	58.584958	7.261033	64.853027
O	55.821873	7.336930	64.200665	O	55.912917	7.304439	64.232678	O	56.184119	6.981068	64.471697
O	56.648668	8.200411	66.305617	O	56.648772	8.249282	66.345747	O	56.990917	7.748011	66.642808
C	54.634215	12.941636	61.407585	C	54.634215	12.941636	61.407585	C	54.634215	12.941636	61.407585
C	54.791156	13.084650	62.920885	C	54.893679	13.078489	62.906907	C	54.590646	13.188162	62.910891
S	56.478971	12.725799	63.536406	S	56.609651	12.658051	63.375440	S	56.242260	13.074650	63.709306
H	56.154785	5.856575	64.872566	H	56.235570	5.805059	64.900814	H	56.461238	5.468302	65.074777
H	50.632069	2.637871	70.833154	H	50.651762	2.620997	70.818863	H	50.674549	2.615908	70.753999

H	51.119092	4.013706	71.842339	H	51.080386	4.019690	71.822699	H	51.023520	3.990640	71.819233
H	52.335388	2.843472	71.288452	H	52.335714	2.864867	71.325057	H	52.322183	2.868028	71.364072
H	51.935876	3.555568	68.898771	H	52.004372	3.535900	68.915591	H	52.121901	3.605531	68.959823
H	50.718932	4.719056	69.443084	H	50.739470	4.675631	69.397562	H	50.818065	4.715779	69.402048
H	52.461868	5.964331	70.723856	H	52.403273	5.991540	70.710926	H	52.394329	5.999850	70.858369
H	53.684124	4.769673	70.222648	H	53.674314	4.822529	70.273479	H	53.695816	4.857185	70.445393
H	55.601537	7.831620	69.262949	H	55.525761	7.934662	69.296324	H	55.819042	7.708768	69.490965
H	54.671457	6.814744	70.364903	H	54.624613	6.884761	70.392913	H	54.798354	6.784307	70.585096
H	55.058900	7.818407	66.973832	H	55.045331	7.850861	66.997444	H	55.350073	7.662895	67.197364
H	53.589367	7.082591	66.429947	H	53.599566	7.090490	66.433053	H	53.833313	7.060821	66.627628
H	54.958079	1.314840	62.197171	H	54.945538	1.325047	62.197733	H	54.899845	1.386760	62.200474
H	54.275211	2.084513	63.643193	H	54.289848	2.094916	63.656286	H	54.406446	2.186071	63.706354
H	56.546710	2.999766	63.207995	H	56.573562	2.976309	63.209712	H	56.774882	2.753563	63.234014
H	57.249518	1.387253	63.179440	H	57.247585	1.352659	63.154700	H	57.209789	1.058632	63.061073
H	56.979891	1.097205	65.554119	H	56.997082	1.034129	65.525619	H	57.107606	0.656707	65.405509
H	55.737201	2.324115	65.667722	H	55.771401	2.275158	65.668980	H	55.922019	1.913029	65.683202
H	55.524262	4.217583	65.085467	H	55.584842	4.175738	65.077126	H	55.773583	3.846005	65.202347
H	59.490887	4.833252	65.618883	H	59.551958	4.739020	65.670205	H	59.763095	4.273579	65.703098
H	58.435842	6.216950	65.226509	H	58.512608	6.138685	65.317497	H	58.762158	5.720206	65.463366
H	60.504171	2.790900	62.032703	H	60.472244	2.786091	62.031820	H	60.478661	2.787674	62.030774
H	59.392551	3.705297	63.072475	H	59.404026	3.726969	63.092679	H	59.402810	3.724447	63.089247
H	61.148569	3.936314	63.220658	H	61.167668	3.918995	63.201850	H	61.163730	3.922984	63.205997
H	61.206266	4.936199	60.888477	H	61.195851	4.919947	60.870075	H	61.188690	4.908034	60.857540
H	59.480561	4.638740	60.705870	H	59.460220	4.656439	60.722172	H	59.451242	4.657988	60.731321
H	58.985283	6.236940	62.579851	H	59.026002	6.252849	62.603229	H	59.086013	6.249808	62.660918
H	59.827488	7.003762	61.226583	H	59.872405	7.021889	61.257240	H	59.822552	7.006168	61.238554
H	61.995933	6.822594	62.520415	H	62.045365	6.795252	62.522274	H	62.060933	6.923442	62.344979
H	61.103027	6.129857	63.883742	H	61.170999	6.059174	63.874918	H	61.352735	6.104349	63.750390
H	60.597969	8.794675	62.693528	H	60.671573	8.776930	62.790672	H	60.501854	8.768402	62.780087
H	61.337277	8.562132	64.194664	H	61.409076	8.476458	64.280515	H	61.489868	8.577186	64.122183
H	54.969507	1.730504	59.016584	H	55.016534	1.721832	59.005958	H	55.022403	1.722288	59.014585
H	55.975898	2.920589	58.165217	H	55.955586	2.963283	58.151049	H	55.952613	2.962464	58.147593
H	54.259931	3.262969	58.465486	H	54.233171	3.229951	58.489329	H	54.229915	3.222829	58.489210
H	56.403636	2.941816	60.658481	H	56.435725	2.980419	60.634370	H	56.433300	2.969569	60.628562
H	54.700848	3.280287	60.949218	H	54.725163	3.240094	60.965503	H	54.726644	3.222100	60.961860
H	54.921077	5.477515	59.768923	H	54.810860	5.447783	59.799217	H	54.814541	5.478957	59.921136
H	56.645980	5.168548	59.510298	H	56.536362	5.219506	59.474565	H	56.533839	5.259199	59.550328
H	57.018471	5.053894	61.976262	H	57.013994	5.131942	61.918792	H	57.060811	4.999977	61.968923
H	55.275271	5.153157	62.259997	H	55.280906	5.148064	62.277003	H	55.337985	4.991089	62.369989
H	57.015958	7.338000	61.282248	H	56.846491	7.428832	61.177917	H	56.865911	7.336232	61.387312
H	56.078628	7.221172	62.740517	H	56.053523	7.253013	62.691951	H	56.196041	7.045043	62.961275
H	61.089067	10.932444	63.926036	H	61.231885	10.838136	64.014077	H	61.150733	10.942625	63.719999
H	56.599883	12.152791	68.164729	H	56.577560	12.263171	68.023487	H	56.806895	11.943394	68.258698
H	52.170593	9.853949	64.178502	H	52.267181	9.832838	63.971540	H	52.237632	9.748641	64.332193
H	56.614342	9.611537	59.577858	H	56.877705	9.550494	59.482844	H	56.516080	9.451632	59.553617
H	60.597020	8.596642	66.481845	H	60.552726	8.595328	66.614976	H	60.839335	8.738909	66.327916
H	58.956820	8.953941	67.077277	H	58.898380	9.011468	67.119589	H	59.242003	9.071356	67.043391
H	60.372101	9.280099	68.109688	H	60.268832	9.338291	68.209439	H	60.723438	9.447261	67.952419
H	61.640963	12.190977	66.057014	H	61.730477	12.111850	66.087097	H	61.754065	12.380202	65.822426
H	61.894632	11.316579	67.554024	H	61.857143	11.355658	67.664334	H	62.109078	11.541590	67.320858
H	59.119017	11.385390	68.392390	H	59.065942	11.496072	68.359981	H	59.389632	11.476344	68.304860
H	54.323258	10.335049	69.039946	H	54.313166	10.422716	68.894757	H	54.518387	9.915618	69.132492
H	53.056321	11.567507	69.246286	H	53.025075	11.639878	69.042711	H	53.310603	11.167682	69.512020
H	54.753515	12.037617	69.370599	H	54.711427	12.141245	69.183812	H	55.027514	11.565728	69.588954
H	53.740298	13.274503	65.932434	H	53.705984	13.261681	65.698006	H	53.912258	13.147502	66.331204
H	54.567129	13.756183	67.433933	H	54.496194	13.809810	67.198625	H	54.770583	13.468799	67.858339
H	52.159586	9.133889	61.649368	H	52.326362	9.151539	61.437784	H	52.142941	8.926312	61.832243
H	54.037056	9.085059	59.666491	H	54.266813	9.101855	59.496835	H	53.917347	8.852325	59.774232

H	59.189496	10.150735	59.454068	H	59.483357	10.036793	59.465680	H	59.143199	9.949433	59.330071
H	61.057555	10.916293	61.297381	H	61.301023	10.794540	61.377708	H	61.066832	10.734906	61.086494
H	54.862812	11.922984	61.085044	H	54.779032	11.909113	61.076915	H	55.060274	11.958280	61.190089
H	54.087178	12.427607	63.446740	H	54.214053	12.439929	63.483052	H	53.933438	12.457584	63.400262
H	54.559016	14.114274	63.231142	H	54.736115	14.115234	63.237644	H	54.188512	14.187200	63.129013
H	52.331153	5.824706	67.903085	H	52.370505	5.785079	67.890599	H	52.454989	5.939381	68.061734
H	58.649530	2.702857	65.670749	H	58.683755	2.614791	65.681082	H	58.837744	2.177277	65.642291
H	59.693572	8.127603	63.914213	H	59.776101	8.066751	63.991686	H	59.880004	7.948910	64.100599
H	55.374140	7.414136	61.201937	H	55.212296	7.417365	61.227054	H	55.235858	7.318372	61.559045
H	53.604471	13.183117	61.095621	H	53.600942	13.241209	61.174566	H	53.621938	12.984924	60.974484
H	55.319249	13.623894	60.884175	H	55.314272	13.585530	60.833375	H	55.253872	13.699895	60.908015
O	53.207742	6.945388	64.613183	O	53.274869	6.975672	64.600483	O	53.526540	6.860405	64.802293
H	54.173652	7.138924	64.432382	H	54.249308	7.133846	64.444435	H	54.516703	6.938485	64.677484
H	52.821810	7.835586	64.469881	H	52.923240	7.873832	64.417179	H	53.238446	7.780848	64.606807
O	56.821767	8.988056	68.810603	O	56.747668	9.122181	68.838647	O	57.133704	8.828789	69.029020
H	56.918087	8.782066	67.838602	H	56.885959	8.875614	67.883376	H	57.234822	8.524765	68.080762
H	56.582553	9.935403	68.782566	H	56.507753	10.066336	68.757274	H	56.894096	9.769406	68.917627
H	54.924045	0.435795	63.734572	H	54.911630	0.434850	63.728511	H	54.781880	0.452789	63.699924
H	52.967246	9.780520	67.117776	H	53.055946	9.766646	66.959137	H	53.023017	9.592331	67.247594
H	52.126721	11.185688	66.397246	H	52.149652	11.119011	66.214479	H	52.260003	11.083331	66.628475
H	59.449815	12.693201	67.224683	H	59.481514	12.744392	67.153702	H	59.565283	12.795965	67.116365

Siroheme (Fe³⁺) with SO₃²⁻

S=1/2			S=3/2			S=5/2					
C	51.422358	3.380522	70.997438	C	51.422358	3.380522	70.997438	C	51.422358	3.380522	70.997438
C	51.717113	4.139652	69.701333	C	51.846597	4.075236	69.701489	C	51.788495	4.084790	69.689535
C	52.774086	5.226159	69.891335	C	53.083391	4.952050	69.889599	C	52.865348	5.150323	69.885800
N	53.057215	5.884799	68.616735	N	53.455861	5.575008	68.620849	N	53.199439	5.770997	68.605441
C	54.061164	6.753637	68.401208	C	54.567212	6.307236	68.414358	C	54.240669	6.595771	68.391229
N	54.887528	7.088698	69.398790	N	55.447285	6.485242	69.408538	N	55.077765	6.896168	69.392355
N	54.234932	7.282362	67.187916	N	54.796480	6.838367	67.214681	N	54.444789	7.110411	67.177656
C	55.076348	1.425184	63.280932	C	55.076348	1.425184	63.280932	C	55.076348	1.425184	63.280932
C	56.461935	1.961461	63.634151	C	56.505939	1.721810	63.727855	C	56.506910	1.773045	63.687453
C	56.673268	2.062349	65.155104	C	56.620426	1.777989	65.261971	C	56.663946	1.867820	65.217721
N	57.725244	3.004383	65.532959	N	57.754154	2.565811	65.737168	N	57.756095	2.740386	65.641109
C	57.590935	4.335803	65.381108	C	57.814601	3.903671	65.588655	C	57.716799	4.076790	65.475136
N	56.397328	4.848169	65.077065	N	56.733499	4.574921	65.186345	N	56.583039	4.656688	65.078227
N	58.635525	5.152667	65.545799	N	58.938221	4.573200	65.853791	N	58.792901	4.830694	65.716719
C	60.333112	3.765595	62.506421	C	60.333112	3.765595	62.506421	C	60.333112	3.765595	62.506421
C	60.256756	4.891209	61.442682	C	60.256756	4.891209	61.442682	C	60.256756	4.891209	61.442682
C	60.012123	6.275551	62.049274	C	60.127506	6.281831	62.074326	C	60.120463	6.284287	62.065289
C	61.113597	6.730773	63.006514	C	61.357763	6.712761	62.875138	C	61.287163	6.678015	62.974167
N	60.822055	8.103763	63.491679	N	61.057361	7.969775	63.607228	N	61.013909	8.011506	63.573600
C	55.161658	2.803979	58.893853	C	55.161658	2.803979	58.893853	C	55.161658	2.803979	58.893853
C	55.522484	3.451533	60.237172	C	55.522484	3.451533	60.237172	C	55.522484	3.451533	60.237172
C	55.865418	4.935700	60.149458	C	55.960420	4.915409	60.154682	C	55.945969	4.915424	60.142666
C	56.141005	5.469506	61.543084	C	56.244135	5.435882	61.554702	C	56.206772	5.448937	61.539142
N	56.320723	6.942775	61.590061	N	56.631282	6.874523	61.602192	N	56.534625	6.897249	61.583138
Fe	56.767126	10.590853	63.885234	Fe	57.339661	10.814731	63.448241	Fe	57.033026	10.919742	63.724756
C	60.168498	10.872079	63.912035	C	60.763687	10.899053	63.500409	C	60.489831	10.873083	63.942334
C	56.667413	11.757834	67.027961	C	57.295112	11.845884	66.652084	C	56.899677	11.620152	67.054833
C	53.430094	9.898938	63.968424	C	54.124553	9.675091	63.737499	C	53.750064	9.829249	63.845404
C	56.853800	9.878681	60.511022	C	57.381118	10.007380	60.129284	C	57.250376	9.945827	60.431005
N	58.153628	11.019915	65.252372	N	58.758763	11.167198	64.830420	N	58.461744	11.071911	65.263927
C	59.525272	10.861515	65.108015	C	60.123231	10.971316	64.699473	C	59.823526	10.884467	65.137216
C	60.186796	10.803609	66.473314	C	60.782819	10.997450	66.070639	C	60.451298	10.772270	66.521167
C	60.028257	9.389328	67.079494	C	60.570572	9.662515	66.822667	C	60.269066	9.338464	67.073987
C	61.652373	11.240351	66.495866	C	62.259538	11.387067	66.071615	C	61.919927	11.190839	66.611632
C	62.748545	10.355318	65.833552	C	63.322233	10.374014	65.558124	C	63.023172	10.249107	66.045059

O	62.452906	9.236254	65.278660	O	62.967624	9.291521	64.970723	O	62.719077	9.260982	65.287709
O	63.910888	10.819892	65.908776	O	64.512932	10.713527	65.759420	O	64.194361	10.552745	66.378842
C	59.219752	11.751405	67.225414	C	59.838063	12.035027	66.731221	C	59.462152	11.685623	67.296234
C	57.920847	11.507065	66.491453	C	58.531892	11.698364	66.057842	C	58.178986	11.461363	66.526459
N	55.308206	10.775146	65.254878	N	55.964187	10.733145	64.936004	N	55.556875	10.704203	65.231467
C	55.462320	11.382379	66.462533	C	56.124087	11.296137	66.162369	C	55.694496	11.238253	66.469403
C	54.122201	11.640199	67.138168	C	54.845646	11.265054	66.981929	C	54.341237	11.407143	67.149073
C	54.110475	11.389176	68.645716	C	55.064446	10.843617	68.436909	C	54.320952	11.046538	68.634235
C	53.747435	13.115643	66.810356	C	54.216576	12.684751	66.887331	C	53.940595	12.895908	66.922392
C	52.340642	13.492273	67.334000	C	52.855532	12.758818	67.626095	C	52.533215	13.210408	67.489456
O	52.289105	14.147166	68.414541	O	52.852822	13.322238	68.757100	O	52.489384	13.819785	68.595679
O	51.353649	13.090439	66.644376	O	51.864204	12.228284	67.038908	O	51.545067	12.809429	66.802993
C	53.220017	10.657865	66.370682	C	54.014239	10.238031	66.194686	C	53.460922	10.469133	66.295512
C	53.988446	10.408380	65.107717	C	54.699478	10.183876	64.866609	C	54.257544	10.305588	65.031991
N	55.430296	9.953991	62.527587	N	56.036731	9.960219	62.199208	N	55.754735	9.974236	62.400030
C	54.099226	9.704003	62.747322	C	54.739729	9.591104	62.477169	C	54.433160	9.678435	62.614557
C	53.460334	9.286500	61.534436	C	54.085413	9.144492	61.287356	C	53.831539	9.251774	61.384107
C	54.417731	9.322035	60.543991	C	54.989482	9.288374	60.251820	C	54.805965	9.327077	60.406663
C	55.639503	9.745605	61.165180	C	56.199213	9.792123	60.821233	C	56.008354	9.782074	61.044985
N	58.220085	10.397970	62.492052	N	58.767946	10.546635	62.090082	N	58.588145	10.511933	62.417780
C	58.053719	10.195625	61.124680	C	58.583483	10.349582	60.720066	C	58.449753	10.282598	61.055544
C	59.305299	10.365688	60.447946	C	59.835802	10.466328	60.040102	C	59.735623	10.385535	60.428095
C	60.234233	10.697563	61.407691	C	60.792415	10.716013	60.996853	C	60.648719	10.672457	61.422039
C	59.539763	10.719059	62.664329	C	60.116691	10.769885	62.258306	C	59.914291	10.748322	62.656734
S	56.995443	8.386361	64.786012	S	57.716257	8.077421	64.992980	S	57.354701	8.166655	64.891797
O	58.349439	7.727306	64.549029	O	58.992386	7.221625	65.167476	O	58.694888	7.414482	64.784144
O	55.982273	7.380968	64.129070	O	56.740430	7.109041	64.188809	O	56.346059	7.196105	64.135938
O	56.694322	8.307076	66.263301	O	57.064665	8.175960	66.370974	O	56.915016	8.046926	66.348260
C	54.634215	12.941636	61.407585	C	54.634215	12.941636	61.407585	C	54.634215	12.941636	61.407585
C	54.882510	13.083917	62.909163	C	55.130251	13.190421	62.827868	C	54.898733	13.202302	62.886624
S	56.600366	12.695863	63.390436	S	56.952549	13.055219	62.972716	S	56.687866	13.132634	63.298346
H	56.278339	5.851414	64.819810	H	56.788933	5.576936	64.890660	H	56.540825	5.666004	64.804877
H	50.653307	2.616501	70.831769	H	50.528595	2.767098	70.833050	H	50.647557	2.623491	70.826512
H	51.060256	4.058531	71.782047	H	51.188878	4.112385	71.783065	H	51.037647	4.093967	71.738802
H	52.322868	2.876834	71.374891	H	52.218421	2.723077	71.373866	H	52.295685	2.877428	71.434478
H	52.067136	3.438412	68.928860	H	52.058831	3.325254	68.924267	H	52.149635	3.349769	68.954694
H	50.794448	4.603046	69.320718	H	51.022111	4.701340	69.327026	H	50.893849	4.558426	69.257655
H	52.426550	5.963994	70.632671	H	52.881384	5.724333	70.650649	H	52.515523	5.912165	70.601561
H	53.701865	4.773076	70.274846	H	53.924283	4.337534	70.247018	H	53.771038	4.684425	70.303896
H	55.592429	7.839067	69.251412	H	56.263666	7.114577	69.275172	H	55.805198	7.626499	69.253197
H	54.673808	6.804915	70.345946	H	55.177484	6.254766	70.356261	H	54.830295	6.645184	70.340702
H	55.120174	7.756297	66.946906	H	55.685018	7.326890	66.991681	H	55.358238	7.540374	66.936156
H	53.704285	6.948816	66.371505	H	54.243256	6.587103	66.387561	H	53.916354	6.787652	66.357792
H	54.964730	1.301607	62.197937	H	55.014933	1.316007	62.192475	H	54.992864	1.294627	62.196239
H	54.288601	2.109130	63.626780	H	54.394116	2.234172	63.578758	H	54.377295	2.218561	63.580466
H	56.589878	2.959183	63.191727	H	56.828686	2.686015	63.309606	H	56.789773	2.736255	63.240682
H	57.249277	1.328652	63.202541	H	57.203501	0.966850	63.340343	H	57.216167	1.031742	63.296242
H	56.944605	1.089968	65.578809	H	56.727383	0.772776	65.682921	H	56.852813	0.881506	65.653601
H	55.737428	2.355065	65.656581	H	55.695737	2.186732	65.699834	H	55.727559	2.222289	65.677647
H	55.593411	4.240010	65.005528	H	55.856122	4.089375	65.060329	H	55.746919	4.099501	64.970407
H	59.554949	4.763351	65.708575	H	59.793629	4.066234	66.041147	H	59.680948	4.383817	65.905086
H	58.548269	6.161614	65.296891	H	58.978935	5.603626	65.668352	H	58.778524	5.846607	65.460646
H	60.452391	2.785532	62.028605	H	60.348232	2.777811	62.030150	H	60.339988	2.777932	62.029330
H	59.413396	3.737489	63.107764	H	59.463073	3.808556	63.175587	H	59.466513	3.810630	63.180399
H	61.180422	3.908134	63.188501	H	61.234698	3.850214	63.124787	H	61.239824	3.845415	63.118207
H	61.187471	4.905076	60.856618	H	61.144465	4.853899	60.794376	H	61.149694	4.853245	60.801495
H	59.448148	4.665988	60.732440	H	59.390707	4.713251	60.788706	H	59.395682	4.711229	60.782761
H	59.061505	6.281013	62.606296	H	59.263905	6.290316	62.758539	H	59.203793	6.328450	62.674105

H	59.919106	7.021438	61.243500	H	59.940355	7.038057	61.294127	H	60.024948	7.042432	61.270830
H	62.094007	6.737539	62.516502	H	62.223192	6.878947	62.224298	H	62.233481	6.725705	62.423350
H	61.180634	6.081393	63.885642	H	61.632419	5.963303	63.624346	H	61.408202	5.971757	63.801982
H	60.798018	8.763641	62.701842	H	60.734979	8.700069	62.958212	H	60.904809	8.719296	62.834046
H	61.502947	8.511831	64.216143	H	61.857953	8.419702	64.153438	H	61.735670	8.402181	64.250522
H	54.919548	1.741931	59.024359	H	54.852264	1.761111	59.036642	H	54.864408	1.756916	59.032342
H	55.995907	2.875481	58.182695	H	56.018202	2.811607	58.206007	H	56.014561	2.824607	58.201733
H	54.290526	3.296905	58.441101	H	54.334607	3.338826	58.407411	H	54.326297	3.332342	58.414408
H	56.373346	2.912143	60.682240	H	56.327125	2.869562	60.713974	H	56.333247	2.876262	60.711511
H	54.680665	3.328688	60.935298	H	54.656339	3.385723	60.913071	H	54.658777	3.381132	60.915610
H	55.022775	5.490264	59.708550	H	55.169120	5.522804	59.689310	H	55.151063	5.509207	59.665936
H	56.736869	5.096794	59.497104	H	56.857673	5.013203	59.524081	H	56.846803	5.018279	59.518588
H	57.041294	5.017906	61.979640	H	57.057906	4.873788	62.032377	H	57.035905	4.917734	62.024764
H	55.300908	5.245093	62.211098	H	55.357372	5.341775	62.193624	H	55.319796	5.321244	62.171414
H	57.205881	7.259548	61.180615	H	57.501063	7.060016	61.093321	H	57.436331	7.113679	61.148127
H	56.259812	7.258539	62.629386	H	56.758307	7.144673	62.651569	H	56.542054	7.188137	62.641555
H	61.253701	10.913311	63.911379	H	61.849187	10.863266	63.494959	H	61.575579	10.852406	63.983602
H	56.634047	12.251246	67.998128	H	57.263207	12.307101	67.636015	H	56.842119	12.041253	68.057759
H	52.355471	9.715025	63.979244	H	53.078268	9.374136	63.798970	H	52.680420	9.616239	63.826260
H	56.863421	9.722443	59.432544	H	57.370037	9.858551	59.050391	H	57.289510	9.768063	59.356237
H	60.632910	8.666493	66.527329	H	61.126629	8.849583	66.352885	H	60.861798	8.622942	66.501117
H	58.982211	9.068959	67.065748	H	59.509430	9.394066	66.864770	H	59.218703	9.032735	67.048818
H	60.373206	9.411776	68.122494	H	60.935250	9.781253	67.852089	H	60.610443	9.319746	68.118004
H	61.751462	12.241804	66.051651	H	62.404166	12.313371	65.494836	H	62.065920	12.169523	66.128738
H	61.964914	11.350085	67.545362	H	62.554430	11.629455	67.102809	H	62.174812	11.341151	67.670377
H	59.146900	11.543186	68.299288	H	59.791365	11.960056	67.823186	H	59.376826	11.436160	68.359751
H	54.394265	10.351792	68.868603	H	55.574503	9.872558	68.477311	H	54.626126	10.002654	68.784632
H	53.102764	11.560529	69.043856	H	54.096298	10.751092	68.944297	H	53.306329	11.167118	69.032991
H	54.785912	12.069274	69.180451	H	55.655864	11.581217	68.993115	H	54.976103	11.701709	69.222481
H	53.777032	13.247606	65.720007	H	54.069232	12.934120	65.826844	H	53.952206	13.098737	65.842308
H	54.500741	13.773215	67.262749	H	54.913305	13.410445	67.324836	H	54.686674	13.537738	67.407455
H	52.408162	9.033683	61.445221	H	53.057220	8.798805	61.239012	H	52.792661	8.958428	61.267230
H	54.303473	9.108786	59.484859	H	54.844930	9.073734	59.197143	H	54.704659	9.116004	59.345802
H	59.449193	10.256649	59.377043	H	59.967948	10.354212	58.968091	H	59.924020	10.255444	59.366381
H	61.289976	10.919846	61.280349	H	61.861599	10.851720	60.865934	H	61.720019	10.823428	61.324413
H	54.772548	11.911571	61.073368	H	54.912426	11.942074	61.060817	H	55.009060	11.961544	61.103285
H	54.206366	12.440518	63.484095	H	54.675804	12.477308	63.526458	H	54.370882	12.472797	63.512364
H	54.711741	14.119544	63.233974	H	54.860049	14.199744	63.164425	H	54.553304	14.201684	63.179709
H	52.445112	5.682196	67.833902	H	52.770976	5.559538	67.872607	H	52.570652	5.610401	67.825941
H	58.648086	2.643860	65.745538	H	58.595058	2.085343	66.035342	H	58.629386	2.324955	65.942265
H	59.860456	8.131577	63.918184	H	60.253399	7.781567	64.278339	H	60.086063	7.960224	64.085851
H	55.569829	7.447908	61.088510	H	55.903288	7.482843	61.185456	H	55.823137	7.475065	61.103350
H	53.604630	13.248236	61.172032	H	53.538029	13.029165	61.368619	H	53.552560	12.976683	61.211402
H	55.318977	13.582452	60.836741	H	55.062159	13.674068	60.710085	H	55.121166	13.703070	60.784044
O	53.385298	6.802888	64.512174	O	54.125905	6.603366	64.452906	O	53.727566	6.727871	64.440959
H	54.315744	7.120891	64.345302	H	55.078891	6.901257	64.379538	H	54.685617	6.993807	64.333411
H	52.860173	7.604564	64.328568	H	53.637613	7.416136	64.224480	H	53.261785	7.563025	64.246096
O	56.816141	9.043222	68.813534	O	57.691126	8.140546	68.915774	O	57.074745	8.811606	68.857901
H	56.919098	8.906913	67.834369	H	57.608333	8.245222	67.921915	H	57.162041	8.650592	67.876154
H	56.569073	9.983054	68.882315	H	57.669694	9.044176	69.272795	H	56.825946	9.750771	68.915587
H	54.896669	0.446754	63.747714	H	54.704046	0.493550	63.729998	H	54.743112	0.491992	63.755322
H	53.124168	9.712599	66.928909	H	54.075977	9.248445	66.674493	H	53.358344	9.489549	66.788884
H	52.220244	11.071227	66.192697	H	52.959201	10.531270	66.129012	H	52.462083	10.890410	66.130781
H	59.522182	12.803673	67.093712	H	60.133952	13.061302	66.457217	H	59.754451	12.745229	67.208127

Siroheme (Fe²⁺) with NO₂⁻

S=0				S=1				S=2			
C	50.353397	-52.121132	49.522288	C	50.353397	-52.121132	49.522288	C	50.353397	-52.121132	49.522288
C	50.567796	-50.635888	49.830888	C	50.413763	-50.597610	49.633585	C	50.474388	-50.600324	49.634689

H	49.226857	-44.276644	49.226599	H	49.002805	-43.882888	48.765256	H	48.931504	-43.962574	49.437490
H	50.325924	-44.825798	50.492204	H	49.927755	-44.608943	50.083128	H	50.016902	-44.744777	50.589475
H	50.677606	-41.067823	50.641592	H	50.483211	-40.895740	50.596753	H	50.716997	-41.086903	51.170046
H	50.473131	-42.524160	51.648967	H	49.992961	-42.398882	51.423138	H	50.321657	-42.623548	51.984517
H	53.286283	-38.409452	45.498177	H	54.020657	-38.233119	45.957385	H	53.552590	-38.451551	45.771044
H	55.993239	-38.112249	45.423067	H	56.725180	-38.172831	46.301526	H	56.257237	-38.241004	45.905909
H	60.035091	-40.307028	48.034058	H	60.177846	-41.186052	48.938422	H	60.040180	-40.742975	48.716386
H	60.247216	-42.354322	49.824515	H	59.954223	-43.519613	50.332176	H	60.088167	-42.946094	50.308258
H	52.534026	-39.533497	49.932618	H	52.624464	-39.548837	49.916740	H	52.627333	-39.573135	49.923476
H	53.347834	-41.229234	51.642245	H	53.024935	-41.235350	51.777712	H	53.025357	-41.212365	51.826863
H	54.138580	-39.930105	52.537403	H	53.835195	-39.979622	52.723626	H	53.829267	-39.933359	52.742895
H	51.177226	-48.193971	49.885324	H	50.928901	-48.148859	49.736975	H	51.120284	-48.196905	49.976592
H	56.066622	-48.921835	43.896662	H	55.331652	-49.530593	44.620882	H	56.050508	-48.908208	44.031131
H	57.679139	-43.726946	46.992213	H	57.202099	-43.753798	46.990110	H	57.490381	-43.657148	47.014680
H	53.418162	-41.875241	45.843429	H	53.433490	-41.658246	45.802499	H	53.304850	-41.939654	45.893129
H	51.937906	-39.141106	51.565285	H	51.886666	-39.008597	51.442836	H	51.884378	-38.996525	51.433354
H	53.305871	-38.238028	50.867099	H	53.423329	-38.300496	50.890320	H	53.422527	-38.301313	50.868809
O	52.157992	-45.267909	46.307346	O	52.179759	-45.601738	45.985373	O	51.839894	-44.505214	46.547156
H	52.809798	-44.923671	46.976373	H	52.699331	-45.123252	46.701050	H	52.658652	-44.497478	47.125035
H	51.291238	-44.919859	46.575203	H	51.411727	-45.991909	46.435264	H	51.243223	-43.847139	46.942153
O	56.628479	-46.888493	48.518151	O	56.371995	-46.761167	48.623307	O	56.496672	-46.759318	48.662371
H	56.519986	-45.914236	48.257507	H	56.197650	-45.820482	48.281130	H	56.385579	-45.800364	48.340525
H	57.099095	-46.880502	49.372057	H	56.764658	-46.641861	49.507833	H	56.970586	-46.701503	49.512154
H	51.917207	-47.996038	41.952943	H	51.659981	-47.964326	42.162158	H	51.906832	-47.998621	41.964857
H	54.694123	-43.795599	53.271108	H	54.045783	-44.161613	53.387673	H	54.319356	-44.345800	53.482142
H	54.167939	-45.383109	52.679952	H	53.296988	-45.604034	52.678494	H	53.757263	-45.860596	52.756973
H	50.665067	-42.922114	47.381842	H	50.733822	-42.529573	47.211351	H	50.283530	-42.473329	47.724052
H	50.022069	-41.474027	48.175010	H	50.154786	-41.055653	48.015870	H	50.070443	-41.054198	48.728202

Siroheme (Fe³⁺) with NO₂⁻

S=1/2			S=3/2			S=5/2					
C	50.353397	-52.121132	49.522288	C	50.353397	-52.121132	49.522288	C	50.353397	-52.121132	49.522288
C	50.630668	-50.630103	49.730113	C	50.654511	-50.642685	49.780482	C	50.625095	-50.631844	49.751008
C	52.117653	-50.289865	49.630498	C	52.140240	-50.315299	49.634507	C	52.088376	-50.262238	49.512500
N	52.313091	-48.847993	49.813523	N	52.358761	-48.880415	49.842559	N	52.277864	-48.818777	49.697249
C	53.431051	-48.174802	49.530842	C	53.475424	-48.215724	49.535040	C	53.403579	-48.150654	49.438982
N	54.508878	-48.804340	49.052943	N	54.532199	-48.852931	49.020070	N	54.482492	-48.788414	48.969530
N	53.483690	-46.845711	49.730241	N	53.548156	-46.889538	49.743947	N	53.470265	-46.824132	49.652732
C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410
C	53.541465	-47.653323	42.953001	C	53.531709	-47.686644	42.938290	C	53.713236	-46.913071	42.751939
C	53.291641	-48.726166	44.015848	C	53.265664	-48.770732	43.986319	C	54.338356	-48.265004	43.101018
N	54.514164	-49.227453	44.641561	N	54.481605	-49.295998	44.605856	N	55.716317	-48.173907	43.580348
C	55.223967	-48.528651	45.535543	C	55.203289	-48.612074	45.501702	C	56.050011	-48.008607	44.863509
N	54.751565	-47.372493	46.010642	N	54.747438	-47.453049	45.986234	N	55.111167	-47.781490	45.790355
N	56.420670	-48.963885	45.951204	N	56.394608	-49.065877	45.911692	N	57.335247	-48.078802	45.244831
C	57.646397	-45.007662	42.604348	C	57.646397	-45.007662	42.604348	C	57.646397	-45.007662	42.604348
C	57.606397	-43.479422	42.863688	C	57.606397	-43.479422	42.863688	C	57.606397	-43.479422	42.863688
C	57.675007	-43.134195	44.359226	C	57.683894	-43.134697	44.357634	C	57.700394	-43.139308	44.357196
C	58.968215	-43.606181	45.011394	C	58.982978	-43.599914	45.001830	C	59.000588	-43.619538	44.988560
N	58.947018	-43.345216	46.485260	N	58.948673	-43.367132	46.479887	N	58.986218	-43.375395	46.464628
C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430
C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930
C	53.159390	-42.477818	43.146884	C	53.159464	-42.486592	43.156935	C	53.191459	-42.482805	43.134022
C	53.881920	-43.327756	44.184124	C	53.884875	-43.348842	44.183494	C	53.897227	-43.343676	44.174182
N	54.398639	-42.510196	45.324823	N	54.410114	-42.554019	45.337946	N	54.443401	-42.551002	45.317337
Fe	55.388211	-41.530480	48.735533	Fe	55.422891	-41.633912	48.896445	Fe	55.479721	-41.237824	48.786455
C	58.199095	-42.785041	50.203463	C	58.252068	-43.004956	50.254163	C	58.272978	-42.740616	50.138036
C	53.476307	-43.529654	50.703268	C	53.519894	-43.691002	50.807634	C	53.519268	-43.511176	50.492234
C	52.584862	-40.605506	47.001477	C	52.605712	-40.737048	47.123226	C	52.704796	-40.452320	46.828728

H	57.473943	-45.223400	41.543223	H	57.463861	-45.223976	41.544993	H	57.453085	-45.225350	41.547108
H	56.867419	-45.521516	43.186288	H	56.874116	-45.522778	43.194157	H	56.878509	-45.521165	43.201192
H	58.615164	-45.443821	42.876116	H	58.618557	-45.442130	42.866601	H	58.620815	-45.441699	42.858465
H	58.431646	-42.986046	42.331119	H	58.427545	-42.985521	42.325145	H	58.420742	-42.984331	42.316281
H	56.678986	-43.059721	42.450192	H	56.675972	-43.060750	42.455825	H	56.670444	-43.063078	42.466549
H	56.838455	-43.629870	44.877032	H	56.853604	-43.634302	44.880922	H	56.870810	-43.633307	44.886799
H	57.566441	-42.048717	44.508606	H	57.571478	-42.050008	44.508066	H	57.598473	-42.054144	44.512980
H	59.841511	-43.092887	44.595123	H	59.849865	-43.066351	44.598438	H	59.870756	-43.102021	44.571462
H	59.106459	-44.684396	44.888796	H	59.137407	-44.673584	44.860879	H	59.137177	-44.696517	44.853054
H	58.970762	-42.329715	46.700217	H	58.930694	-42.356803	46.710045	H	58.992435	-42.362059	46.682126
H	59.765598	-43.753821	46.947225	H	59.777993	-43.755021	46.940415	H	59.811759	-43.776527	46.920059
H	51.424472	-43.515631	40.244821	H	51.428579	-43.516862	40.243791	H	51.400339	-43.515530	40.260157
H	52.541562	-42.137649	40.335809	H	52.540095	-42.134425	40.337433	H	52.547291	-42.160461	40.319269
H	51.012836	-42.103213	41.238835	H	51.009760	-42.106552	41.237820	H	51.030906	-42.081651	41.240347
H	53.318124	-44.085880	41.735003	H	53.319003	-44.083973	41.733307	H	53.295488	-44.110630	41.735213
H	51.808348	-44.059585	42.632687	H	51.808535	-44.063298	42.628393	H	51.796653	-44.031009	42.651192
H	52.382417	-41.870802	43.636429	H	52.382360	-41.886641	43.654624	H	52.434188	-41.851107	43.622580
H	53.865326	-41.780973	42.669671	H	53.863999	-41.783769	42.686354	H	53.912929	-41.809397	42.646495
H	54.739519	-43.849852	43.742906	H	54.739343	-43.867875	43.732360	H	54.738475	-43.889590	43.729351
H	53.213240	-44.078351	44.622345	H	53.216680	-44.104357	44.614188	H	53.214126	-44.081978	44.611536
H	55.049076	-41.774478	45.019256	H	55.052521	-41.808064	45.042023	H	55.107859	-41.827383	45.015351
H	54.894385	-43.083865	46.055912	H	54.917677	-43.150075	46.047311	H	54.937906	-43.162852	46.024569
H	59.096840	-43.201914	50.661729	H	59.152408	-43.442197	50.687914	H	59.159038	-43.130909	50.653296
H	52.856267	-44.072017	51.414420	H	52.902637	-44.234443	51.520118	H	52.881575	-44.081650	51.165721
H	51.695202	-40.285993	46.461110	H	51.715096	-40.412904	46.587945	H	51.825224	-40.110044	46.284952
H	57.936568	-39.009509	45.953022	H	57.947496	-39.031583	46.179901	H	58.126638	-39.022786	45.800888
H	57.956855	-45.892872	50.637455	H	58.015393	-46.110538	50.647864	H	58.113093	-45.802094	50.451016
H	56.192164	-45.834466	50.296226	H	56.250020	-46.049857	50.308667	H	56.363254	-45.815760	50.096412
H	56.784399	-46.522165	51.827849	H	56.844370	-46.758604	51.829387	H	56.977374	-46.541823	51.608289
H	57.950070	-43.175094	53.204598	H	58.017733	-43.430989	53.247831	H	58.057416	-43.178953	53.041506
H	57.439656	-44.759941	53.761053	H	57.509193	-45.022396	53.787076	H	57.389365	-44.697484	53.682728
H	51.469628	-45.139150	48.682116	H	51.416679	-45.257234	48.809282	H	51.591013	-44.900674	48.236469
H	49.835381	-44.624606	49.155235	H	49.818166	-44.703397	49.350283	H	49.920247	-44.497915	48.709861
H	51.007578	-45.007564	50.412907	H	51.028572	-45.122241	50.559141	H	51.057118	-45.013684	49.949922
H	50.931200	-41.236374	50.450362	H	51.039200	-41.340855	50.595838	H	50.942583	-41.320407	50.561077
H	50.923474	-42.677193	51.502439	H	50.982624	-42.783069	51.645099	H	50.939870	-42.914869	51.361081
H	53.094259	-38.502950	45.151552	H	53.109940	-38.596526	45.312248	H	53.307466	-38.464830	44.827869
H	55.764196	-38.062894	44.814465	H	55.775728	-38.089516	45.040803	H	55.981413	-38.077394	44.546696
H	60.099021	-39.838368	47.187149	H	60.115756	-39.883508	47.394213	H	60.280663	-39.831765	47.124934
H	60.568382	-41.569859	49.248400	H	60.606315	-41.717337	49.357937	H	60.692230	-41.522101	49.216158
H	52.430636	-39.552664	49.976328	H	52.553316	-39.563839	49.936237	H	52.554454	-39.576146	49.940526
H	53.792230	-41.131499	51.435119	H	53.683262	-41.136999	51.566153	H	53.947153	-41.022687	51.484646
H	54.486022	-39.739435	52.277397	H	54.262907	-39.750570	52.500041	H	54.392352	-39.587815	52.422665
H	51.538673	-48.322447	50.207908	H	51.598734	-48.350774	50.258571	H	51.488621	-48.287140	50.051394
H	54.950394	-50.051450	44.243021	H	54.906779	-50.121272	44.197523	H	56.469925	-48.268034	42.908755
H	58.085565	-43.760748	46.930590	H	58.095967	-43.820524	46.907952	H	58.128063	-43.808742	46.901129
H	53.622409	-42.012931	45.812707	H	53.636885	-42.076516	45.847840	H	53.684858	-42.041055	45.817251
H	52.053314	-39.325833	51.702285	H	51.958510	-39.298447	51.594755	H	52.006573	-39.430171	51.628720
H	53.108743	-38.169169	50.856607	H	53.137742	-38.175353	50.874904	H	52.992370	-38.144249	50.893025
O	52.513342	-45.621971	46.167901	O	52.531595	-45.676464	46.175351	O	52.826958	-46.049759	45.935010
H	53.079120	-45.229110	46.875851	H	53.118548	-45.298667	46.876522	H	53.315818	-45.579878	46.654560
H	51.635141	-45.757684	46.561478	H	51.655275	-45.790905	46.580167	H	51.934462	-46.227324	46.277072
O	56.949900	-47.345562	48.266152	O	56.979683	-47.430572	48.205563	O	56.977726	-47.430908	48.097524
H	56.922729	-46.357180	48.128493	H	56.954843	-46.441404	48.069561	H	56.948491	-46.433615	48.039817
H	57.622471	-47.485289	48.956635	H	57.657105	-47.574004	48.891468	H	57.653569	-47.634906	48.768484
H	51.567152	-47.852483	42.056747	H	51.550238	-47.833026	42.047059	H	52.055589	-47.775374	41.632526
H	55.411425	-43.364869	52.995635	H	55.478678	-43.644061	53.075757	H	55.350935	-43.533344	52.858493
H	54.920302	-45.003930	52.512069	H	54.977582	-45.260097	52.531412	H	54.965131	-45.149410	52.233294

H	51.105659	-43.172429	47.239245	H	51.110790	-43.297035	47.379205	H	50.925658	-42.743535	47.096030
H	50.276138	-41.801342	48.005479	H	50.301314	-41.914425	48.150053	H	50.346302	-41.411986	48.099931

Table S7. Cartesian coordinates (Å) of the siroheme species (Fe²⁺ & Fe³⁺) without ligands (and without the cubane cluster) optimized at DFT (BP86 functional) using TZ2P basis sets. S is the spin state of the species.

Siroheme (Fe ²⁺) without HSO ₃ ⁻											
S=0				S=1				S=2			
C	50.428910	4.480310	71.588390	C	50.428910	4.480310	71.588390	C	50.428910	4.480310	71.588390
C	51.181491	5.624492	70.909137	C	51.534437	5.428793	71.129468	C	51.610530	5.332681	71.122971
C	50.440593	6.115249	69.660182	C	51.054217	6.301569	69.966918	C	51.136957	6.514936	70.270837
N	51.208828	7.072052	68.860254	N	52.093792	7.150449	69.387841	N	52.223723	7.270762	69.642840
C	52.246991	6.746760	68.090505	C	52.993590	6.746167	68.490213	C	52.849522	6.894666	68.529094
N	52.528980	5.451683	67.863668	N	53.007575	5.467511	68.086874	N	52.477887	5.758867	67.891061
N	53.009716	7.688450	67.520599	N	53.871231	7.623566	67.983052	N	53.821941	7.653088	68.010620
C	52.322910	2.353310	63.305390	C	52.322910	2.353310	63.305390	C	52.322910	2.353310	63.305390
C	53.591862	2.984461	63.874089	C	53.601662	2.974218	63.866024	C	53.485053	3.152182	63.895914
C	53.355115	3.575725	65.264038	C	53.312894	3.863007	65.074637	C	53.019161	4.110582	64.990852
N	54.570164	4.160079	65.854775	N	54.545160	4.340827	65.735726	N	54.132610	4.735869	65.743807
C	55.054943	5.369094	65.492051	C	55.247909	5.435643	65.301044	C	54.879654	5.796483	65.187392
N	54.270161	6.359423	65.060719	N	54.550953	6.559486	65.016841	N	54.179382	6.952101	64.986184
N	56.355043	5.646332	65.652370	N	56.558414	5.430116	65.247415	N	56.158584	5.748602	64.992620
C	57.721910	3.753310	61.692390	C	57.721910	3.753310	61.692390	C	57.721910	3.753310	61.692390
C	57.681910	4.934310	60.688390	C	57.681910	4.934310	60.688390	C	57.681910	4.934310	60.688390
C	57.442737	6.296033	61.341411	C	57.762717	6.304544	61.371910	C	57.683876	6.305223	61.382037
C	58.596565	6.787800	62.204556	C	59.160390	6.602589	61.900044	C	59.069794	6.677475	61.891886
N	58.219822	8.088913	62.833764	N	59.163622	7.871339	62.684279	N	59.031624	7.960387	62.662313
C	51.935910	3.947310	59.008390	C	51.935910	3.947310	59.008390	C	51.935910	3.947310	59.008390
C	52.628910	4.440310	60.285390	C	52.628910	4.440310	60.285390	C	52.628910	4.440310	60.285390
C	52.688189	5.962325	60.465300	C	51.942044	5.639653	60.944060	C	51.772764	5.475893	61.022423
C	53.875337	6.298266	61.359298	C	52.929933	6.399714	61.815287	C	52.601376	6.359548	61.937695
N	53.797801	7.634224	62.001635	N	52.245017	7.442492	62.633510	N	51.721978	7.265952	62.735501
Fe	54.351170	10.698689	64.780632	Fe	53.901461	10.445826	64.898278	Fe	53.555941	10.512934	65.147684
C	57.618677	10.601724	65.740152	C	57.288628	10.360067	64.836887	C	56.990300	10.460878	65.437068
C	53.436536	11.038217	67.973488	C	53.948268	10.962047	68.218195	C	53.280260	10.742489	68.525300
C	51.150824	10.001880	63.869467	C	50.544201	9.767234	65.042462	C	50.166453	9.920782	64.916581
C	55.296955	10.978001	61.505271	C	53.786221	10.412587	61.463163	C	53.846270	10.085235	61.702292
N	55.301916	10.566905	66.487843	N	55.320894	10.462070	66.264857	N	54.934108	10.472054	66.737875
C	56.667327	10.334392	66.680465	C	56.688093	10.286548	66.056998	C	56.307552	10.518135	66.624865
C	56.913936	9.915833	68.125831	C	57.413601	10.124812	67.388245	C	56.964869	10.649965	68.004656
C	56.525795	8.430634	68.333867	C	57.301280	8.687595	67.952941	C	57.419923	9.257597	68.484974
C	58.326584	10.185795	68.669982	C	58.863298	10.617005	67.402586	C	58.112286	11.697554	68.079192
C	59.363273	9.109256	68.396220	C	60.038459	9.780247	66.894222	C	59.486438	11.147840	67.761389
O	59.417687	8.585858	67.138098	O	59.894730	8.689617	66.130217	O	60.300626	10.910180	68.822586
O	60.138608	8.691978	69.232885	O	61.172944	10.135778	67.186034	O	59.895474	10.888919	66.644665
C	55.831733	10.782351	68.796649	C	56.492482	11.019448	68.249212	C	55.767970	11.134665	68.849539
C	54.774142	10.799947	67.722686	C	55.162284	10.812519	67.575332	C	54.574401	10.750183	68.017747
N	52.651136	10.498277	65.730175	N	52.533964	10.217869	66.377890	N	51.996761	10.137718	66.538355
C	52.437710	10.853003	67.038070	C	52.719741	10.654088	67.650542	C	52.086984	10.496069	67.835175
C	50.961022	11.003075	67.354282	C	51.395239	10.843994	68.369217	C	50.716077	10.786955	68.433813
C	50.575253	10.660821	68.792809	C	51.429244	10.634734	69.880952	C	50.515440	10.361593	69.884619
C	50.573377	12.477731	67.041280	C	50.942872	12.300422	68.044734	C	50.546066	12.330741	68.279604
C	49.068214	12.734887	67.293559	C	49.542330	12.600619	68.636052	C	49.146805	12.804032	68.745904
O	48.763381	13.353643	68.352056	O	49.506686	13.292042	69.691989	O	49.080795	13.333022	69.892285
O	48.265580	12.273720	66.424826	O	48.552489	12.100363	68.019057	O	48.185287	12.596434	67.946335
C	50.371719	10.061520	66.286613	C	50.523245	9.841769	67.585169	C	49.804864	10.039774	67.439494
C	51.409057	10.153094	65.202078	C	51.195812	9.879344	66.240795	C	50.658969	9.997480	66.198343
N	53.432874	10.477579	63.051679	N	52.467692	10.198046	63.540422	N	52.256863	10.013073	63.584481
C	52.095035	10.200124	62.840327	C	51.120257	9.990470	63.774809	C	50.882045	9.988731	63.693316

C	51.793974	10.172226	61.444420	C	50.386209	10.008187	62.546604	C	50.291827	10.038437	62.387546
C	52.963136	10.466206	60.773386	C	51.293170	10.234882	61.532288	C	51.327123	10.096415	61.470479
C	53.974511	10.662538	61.769451	C	52.584168	10.333327	62.145339	C	52.550724	10.077673	62.217679
N	56.099554	10.806351	63.821291	N	55.263197	10.279186	63.432512	N	55.139329	10.055454	63.821342
C	56.295963	11.059362	62.458925	C	55.039114	10.389928	62.058332	C	55.037682	10.109927	62.431054
C	57.677195	11.335389	62.200607	C	56.278720	10.567039	61.370118	C	56.329138	10.373248	61.867678
C	58.333664	11.248186	63.411719	C	57.267072	10.595319	62.332253	C	57.203764	10.528696	62.925605
C	57.351497	10.911981	64.393042	C	56.619615	10.420788	63.595976	C	56.446768	10.333573	64.129220
C	52.934910	13.851310	62.600390	C	52.934910	13.851310	62.600390	C	52.934910	13.851310	62.600390
C	52.753513	13.483412	64.068282	C	52.467665	13.415443	63.985534	C	52.271690	13.391892	63.896397
S	54.277589	12.910067	64.904999	S	53.829340	12.758476	65.020770	S	53.479388	12.795276	65.151417
H	54.835282	7.153116	64.551765	H	55.025287	7.370680	64.627441	H	54.629662	7.737067	64.512213
H	50.957426	4.146734	72.489292	H	50.767523	3.859938	72.426412	H	50.772273	3.648548	72.215220
H	50.329165	3.616703	70.916000	H	50.119301	3.809096	70.775711	H	49.882728	4.058145	70.733286
H	49.418573	4.790367	71.887816	H	49.542508	5.036913	71.920043	H	49.720075	5.076282	72.179289
H	51.308778	6.469616	71.599527	H	51.855217	6.080339	71.953677	H	52.173400	5.720329	71.983732
H	52.193067	5.293012	70.631942	H	52.423032	4.854081	70.826884	H	52.316791	4.713219	70.548807
H	50.144043	5.269525	69.020345	H	50.623819	5.682561	69.165113	H	50.446226	6.178822	69.483281
H	49.509166	6.620310	69.936921	H	50.253542	6.971700	70.300122	H	50.574924	7.225188	70.886763
H	53.438223	5.173140	67.506661	H	53.718150	5.122592	67.436953	H	53.156100	5.367532	67.203005
H	51.983208	4.733613	68.321394	H	52.490962	4.772642	68.611088	H	51.980349	5.064633	68.440107
H	53.580609	7.432347	66.713037	H	54.426940	7.355434	67.177405	H	54.122316	7.472712	67.050208
H	52.834244	8.683587	67.672189	H	53.718946	8.628861	68.102520	H	53.857789	8.638437	68.295868
H	52.508131	1.930469	62.311573	H	52.539815	1.725209	62.433864	H	52.669226	1.680376	62.512143
H	51.514713	3.091836	63.215730	H	51.602626	3.124003	62.997195	H	51.556110	3.013359	62.877219
H	53.957380	3.777020	63.203590	H	54.119258	3.564586	63.093756	H	54.012409	3.714376	63.109616
H	54.393793	2.234877	63.937239	H	54.299629	2.180013	64.169616	H	54.224291	2.461356	64.329049
H	53.008129	2.800531	65.957746	H	52.735218	3.309682	65.825550	H	52.402536	3.567263	65.720104
H	52.568529	4.341256	65.240530	H	52.706685	4.729482	64.789733	H	52.382624	4.905439	64.584518
H	53.297397	6.196985	64.788588	H	53.541475	6.630131	65.193258	H	53.166774	7.001694	65.151367
H	57.029318	4.936417	65.906731	H	57.033831	4.546572	65.404121	H	56.535615	4.812504	65.149996
H	56.675190	6.561087	65.336909	H	57.163823	6.375897	65.112769	H	57.258261	6.936313	65.047170
H	57.828619	2.798588	61.163611	H	57.623650	2.793158	61.170974	H	57.695601	2.791042	61.165825
H	56.792640	3.714863	62.279361	H	56.896198	3.836849	62.413372	H	56.856471	3.798728	62.368118
H	58.562162	3.841026	62.393306	H	58.662647	3.729448	62.257942	H	58.631545	3.770938	62.307607
H	58.616638	4.958685	60.108321	H	58.499715	4.834242	59.959282	H	58.530792	4.868118	59.991872
H	56.877310	4.754095	59.961307	H	56.746768	4.882071	60.113765	H	56.772460	4.850808	60.078070
H	56.550098	6.239511	61.979389	H	57.042539	6.343555	62.204582	H	56.970578	6.294354	62.221796
H	57.236172	7.048798	60.565137	H	57.476296	7.097798	60.664945	H	57.346774	7.083628	60.681356
H	59.516543	6.920741	61.623575	H	59.876507	6.691102	61.074996	H	59.768575	6.801663	61.057400
H	58.807471	6.090360	63.022974	H	59.513919	5.816318	62.576787	H	59.474457	5.917394	62.569498
H	58.890649	8.379006	63.550350	H	60.116824	8.173179	62.905221	H	59.969588	8.353334	62.780877
H	57.184266	8.012116	63.283655	H	58.598002	7.732509	63.660928	H	58.604646	7.817740	63.655576
H	51.921589	2.851010	58.971413	H	52.460538	3.079644	58.589366	H	52.544496	3.195746	58.490237
H	52.460339	4.311042	58.114519	H	51.918873	4.736935	58.245095	H	51.762967	4.781417	58.315538
H	50.896829	4.300346	58.953612	H	50.896936	3.649244	59.207568	H	50.962409	3.491793	59.237276
H	53.659505	4.047691	60.284538	H	53.663266	4.722852	60.030436	H	53.594456	4.896008	60.015585
H	52.143475	4.002432	61.167521	H	52.709749	3.621111	61.011342	H	52.856879	3.598121	60.951159
H	51.752665	6.331788	60.910619	H	51.080362	5.307769	61.543914	H	50.980237	4.972744	61.597961
H	52.802519	6.469953	59.496897	H	51.552030	6.324030	60.175672	H	51.266624	6.121997	60.288139
H	54.806117	6.248807	60.787056	H	53.683160	6.907463	61.202317	H	53.280846	7.001293	61.365667
H	53.952237	5.573031	62.180528	H	53.454791	5.736890	62.514766	H	53.202396	5.782524	62.648349
H	53.692284	8.410474	61.324863	H	51.543060	7.977916	62.086841	H	51.018124	7.736211	62.142440
H	54.663110	7.828370	62.626814	H	52.884949	8.179472	62.984083	H	52.241803	8.063959	63.165117
H	58.664204	10.678651	66.039515	H	58.375707	10.364306	64.796026	H	58.067762	10.622285	65.489293
H	53.149900	11.310112	68.987199	H	53.960973	11.315471	69.246894	H	53.179265	11.049330	69.565810
H	50.120830	9.808029	63.571188	H	49.472630	9.576409	65.070500	H	49.081927	9.865478	64.824849
H	55.573280	11.153731	60.465982	H	53.743854	10.514460	60.379280	H	53.939639	10.150699	60.617994

H	57.125371	7.753797	67.715025	H	57.695958	7.926698	67.274330	H	58.192683	8.840670	67.827276
H	55.469546	8.275212	68.087923	H	56.254491	8.443089	68.166413	H	56.570248	8.562635	68.486514
H	56.672712	8.153113	69.386292	H	57.852371	8.630006	68.901132	H	57.818647	9.308005	69.507333
H	58.710438	11.139447	68.276069	H	58.934555	11.577258	66.869010	H	57.902481	12.512642	67.376362
H	58.284977	10.286562	69.760287	H	59.137080	10.842876	68.442219	H	58.116412	12.126460	69.089451
H	51.098735	9.764249	69.156535	H	52.016578	9.753025	70.176764	H	50.611227	9.273927	69.989551
H	49.493952	10.503331	68.875818	H	50.413874	10.525182	70.276645	H	49.511411	10.644513	70.222587
H	50.840634	11.472119	69.481241	H	51.885065	11.492900	70.389374	H	51.229619	10.852386	70.558124
H	50.809918	12.688829	65.990706	H	50.921176	12.429157	66.953896	H	50.698875	12.596751	67.223721
H	51.179320	13.136727	67.675178	H	51.683119	12.993160	68.463059	H	51.321520	12.826059	68.877232
H	50.308240	9.029335	66.674769	H	50.591459	8.835812	68.031601	H	49.599799	9.019410	67.805862
H	50.810629	9.976476	61.027031	H	49.310231	9.881598	62.469188	H	49.224560	10.052974	62.186112
H	53.121493	10.563199	59.703389	H	51.106027	10.319809	60.466195	H	51.254733	10.151461	60.388103
H	58.089981	11.577110	61.225465	H	56.380061	10.693742	60.296320	H	56.533583	10.492189	60.807299
H	59.390669	11.396302	63.615671	H	58.327876	10.794376	62.198235	H	58.248757	10.826954	62.892066
H	53.248213	12.981036	62.014765	H	53.379300	13.005202	62.061840	H	53.480696	13.018598	62.136013
H	51.985169	12.709287	64.185778	H	51.696145	12.639350	63.906732	H	51.558872	12.581517	63.699209
H	52.417385	14.355205	64.648811	H	52.028344	14.262806	64.529397	H	51.714006	14.217581	64.358115
H	50.973030	8.058610	68.934835	H	52.146601	8.117835	69.696986	H	52.515560	8.147317	70.065468
H	55.271508	3.483630	66.148331	H	55.158439	3.574373	66.011007	H	54.773911	4.013733	66.075162
H	58.182541	8.863201	62.155091	H	58.704282	8.633451	62.165649	H	58.449995	8.672160	62.194503
H	52.962118	7.652222	62.618268	H	51.777061	7.055387	63.480252	H	51.238244	6.789141	63.513523
H	51.990846	14.230364	62.179548	H	52.091650	14.236014	62.006617	H	52.180758	14.212147	61.885034
H	53.699360	14.631320	62.485730	H	53.692968	14.642879	62.673525	H	53.649080	14.664266	62.788701
O	51.731534	7.076108	63.976517	O	51.675429	6.946751	65.315118	O	51.290810	7.024786	65.472736
H	51.483160	8.015143	64.190165	H	51.347562	7.875544	65.481413	H	50.912524	7.930041	65.604241
H	50.903316	6.670416	63.665867	H	51.004137	6.365937	65.712942	H	51.251330	6.576815	66.343546
O	55.812403	7.955476	63.770030	O	57.901727	7.562181	64.912076	O	58.033524	7.610037	65.093756
H	55.745969	8.924706	63.959546	H	57.286075	8.324452	64.893571	H	57.633594	8.466087	65.365355
H	58.750316	9.024253	66.558871	H	58.977949	8.359293	65.811653	H	59.866624	11.187143	69.652015
H	51.963644	1.542046	63.952760	H	51.832304	1.722969	64.058921	H	51.838585	1.741032	64.077758
H	55.476416	10.377675	69.751729	H	56.489352	10.753217	69.312365	H	55.751361	10.704237	69.858328
H	56.204460	11.805981	68.966422	H	56.783183	12.078520	68.154987	H	55.779937	12.230417	68.957469
H	49.375377	10.383894	65.964091	H	49.474863	10.156362	67.549380	H	48.852876	10.560970	67.289516

Siroheme (Fe³⁺) without HSO₃⁻

S=1/2			S=3/2			S=5/2					
C	50.428910	4.480310	71.588390	C	50.428910	4.480310	71.588390	C	50.428910	4.480310	71.588390
C	51.603290	5.365149	71.156941	C	51.571861	5.474672	71.367139	C	51.438572	5.424297	70.939070
C	51.116855	6.586219	70.366865	C	51.547797	6.047026	69.945752	C	51.266832	5.485690	69.418678
N	52.187994	7.444068	69.839526	N	52.555557	7.084224	69.700086	N	52.328453	6.266678	68.752525
C	52.814625	7.236363	68.680666	C	53.799288	6.874964	69.264689	C	53.609901	5.833520	68.711140
N	52.581011	6.107337	67.989094	N	54.274052	5.631889	69.124857	N	53.895736	4.541202	68.858899
N	53.653776	8.158719	68.178867	N	54.568614	7.909876	68.884928	N	54.577681	6.708408	68.430886
C	52.322910	2.353310	63.305390	C	52.322910	2.353310	63.305390	C	52.322910	2.353310	63.305390
C	53.755600	2.783649	63.611471	C	53.560607	2.896215	64.015810	C	53.735932	2.838932	63.659261
C	54.005325	2.813738	65.124653	C	53.233041	3.430879	65.412839	C	53.798431	3.642864	64.965955
N	55.244658	3.493529	65.502237	N	54.425734	3.909661	66.112949	N	55.167923	4.046237	65.309755
C	55.349737	4.813276	65.643429	C	54.903417	5.159250	66.053141	C	55.767176	5.213851	65.000409
N	54.255701	5.604162	65.451419	N	54.154523	6.192256	65.665514	N	55.031026	6.308031	64.735800
N	56.481055	5.402082	66.020010	N	56.171538	5.407102	66.455668	N	57.096037	5.291413	64.973558
C	57.721910	3.753310	61.692390	C	57.721910	3.753310	61.692390	C	57.721910	3.753310	61.692390
C	57.681910	4.934310	60.688390	C	57.681910	4.934310	60.688390	C	57.681910	4.934310	60.688390
C	56.696497	6.043220	61.088819	C	56.767356	6.081911	61.137105	C	58.117783	6.270985	61.290763
C	56.863387	6.524167	62.531255	C	57.062681	6.581415	62.552666	C	59.580108	6.281313	61.726288
N	56.040324	7.705502	62.878598	N	56.330267	7.807870	62.930687	N	59.909827	7.557587	62.402894
C	51.935910	3.947310	59.008390	C	51.935910	3.947310	59.008390	C	51.935910	3.947310	59.008390
C	52.628910	4.440310	60.285390	C	52.628910	4.440310	60.285390	C	52.628910	4.440310	60.285390
C	51.865009	5.650112	60.831973	C	51.699143	5.426648	60.998562	C	51.646503	5.306518	61.083105

C	52.287076	6.073036	62.224297	C	52.209952	5.963261	62.322773	C	52.224246	5.899521	62.354051
N	51.437013	7.198577	62.718549	N	51.138377	6.789607	62.977980	N	51.132290	6.488240	63.200167
Fe	54.630107	10.970227	64.865941	Fe	54.312766	10.898170	65.107092	Fe	53.451757	10.175449	64.735034
C	58.009370	10.765338	65.408685	C	57.732948	11.175272	64.952934	C	56.880462	10.203279	64.645900
C	54.158234	11.568776	68.138760	C	54.436693	11.447392	68.433834	C	53.611268	9.817544	68.184199
C	51.285252	10.428562	64.441822	C	51.061684	9.836705	65.408339	C	50.046485	9.616846	64.922733
C	55.149938	10.682401	61.499890	C	54.173532	10.495934	61.712700	C	53.385522	9.483251	61.341386
N	55.828851	10.966534	66.468314	N	55.826721	11.077689	66.457318	N	55.005111	9.811173	66.160712
C	57.208746	10.745547	66.507154	C	57.195232	11.126587	66.200848	C	56.357920	9.953443	65.886100
C	57.664557	10.573274	67.952440	C	57.962708	11.178984	67.519331	C	57.175239	9.776799	67.170080
C	57.379422	9.126967	68.429163	C	58.094130	9.753862	68.111498	C	57.463779	8.275821	67.414675
C	59.116426	10.987348	68.254941	C	59.316955	11.909489	67.481323	C	58.433105	10.642513	67.293430
C	60.186859	9.915121	68.135552	C	60.565947	11.099308	67.170670	C	59.764952	10.343377	66.603693
O	60.173293	9.107958	67.037417	O	60.508034	10.159925	66.185223	O	59.930154	9.362465	65.700933
O	61.057547	9.751518	68.964318	O	61.619026	11.267476	67.748579	O	60.729086	11.034900	66.886538
C	56.641859	11.501823	68.630515	C	56.921555	11.937192	68.363789	C	56.114838	10.211244	68.202241
C	55.453276	11.346718	67.724906	C	55.634128	11.465607	67.749495	C	54.820955	9.892650	67.501513
N	53.037752	10.913603	66.074343	N	53.045362	10.525693	66.652708	N	52.055037	9.576163	66.317315
C	53.031113	11.329437	67.375164	C	53.243789	10.962830	67.926600	C	52.331720	9.762630	67.634735
C	51.630037	11.569931	67.903584	C	51.959373	10.964835	68.732339	C	51.087452	10.118389	68.432295
C	51.401484	11.141805	69.351432	C	52.116881	10.637710	70.216055	C	50.979473	9.466277	69.808535
C	51.373065	13.096123	67.725681	C	51.363700	12.393410	68.549726	C	51.148865	11.673457	68.552322
C	49.899836	13.456856	68.053757	C	49.965630	12.498796	69.226168	C	49.869495	12.237687	69.221401
O	49.677324	13.940253	69.196213	O	49.923391	13.095897	70.333179	O	49.958986	12.547247	70.439905
O	49.051584	13.200900	67.147163	O	49.007882	11.946559	68.606279	O	48.837761	12.313508	68.491402
C	50.801359	10.756730	66.897998	C	51.126464	9.950782	67.931529	C	49.971363	9.695535	67.459938
C	51.715746	10.673896	65.713247	C	51.741172	10.062827	66.569881	C	50.672144	9.638419	66.135422
N	53.474133	10.540009	63.310749	N	52.924708	10.236617	63.828509	N	52.009931	9.556132	63.403575
C	52.107669	10.385987	63.302088	C	51.603097	9.979525	64.113423	C	50.653445	9.539843	63.647806
C	51.624716	10.190771	61.967695	C	50.847864	9.843019	62.908633	C	49.941592	9.373621	62.416675
C	52.723988	10.249513	61.135129	C	51.736901	10.001160	61.859307	C	50.886758	9.290789	61.409670
C	53.860392	10.481147	61.965347	C	53.015789	10.244434	62.434053	C	52.170359	9.423361	62.022740
N	56.239238	10.798022	63.700560	N	55.664432	10.843904	63.640550	N	54.875483	9.824102	63.267470
C	56.258408	10.855657	62.301725	C	55.403305	10.777761	62.269051	C	54.635976	9.703895	61.901040
C	57.608080	10.963496	61.832273	C	56.614344	10.978913	61.530805	C	55.860918	9.908786	61.182522
C	58.416523	10.957127	62.940561	C	57.617128	11.155541	62.451960	C	56.833903	10.182679	62.115908
C	57.554777	10.857044	64.080116	C	57.010405	11.073748	63.747653	C	56.204221	10.116385	63.404739
C	52.934910	13.851310	62.600390	C	52.934910	13.851310	62.600390	C	52.934910	13.851310	62.600390
C	52.997641	13.672953	64.115534	C	52.499573	13.510246	64.022940	C	52.192867	13.052663	63.667998
S	54.618574	13.076089	64.710350	S	53.932968	13.161245	65.112330	S	53.330661	12.396590	64.961890
H	54.448174	6.614927	65.379054	H	54.645634	7.106873	65.642363	H	55.513322	7.168170	64.496340
H	50.784819	3.616480	72.161734	H	50.457215	4.081729	72.609075	H	50.563395	4.461861	72.676219
H	49.872916	4.105536	70.718242	H	50.495638	3.632126	70.893085	H	50.548455	3.453424	71.215898
H	49.727389	5.038383	72.222118	H	49.453442	4.962804	71.441652	H	49.397243	4.796646	71.383528
H	52.167868	5.710047	72.034435	H	51.493465	6.306816	72.080950	H	51.332991	6.439737	71.346624
H	52.309892	4.777372	70.550288	H	52.540916	4.989500	71.559591	H	52.461285	5.097506	71.177700
H	50.484073	6.275822	69.522675	H	51.683510	5.255599	69.195179	H	51.237977	4.482980	68.969768
H	50.495541	7.225456	71.004103	H	50.573171	6.510502	69.747414	H	50.317149	5.961370	69.148123
H	53.146958	5.906748	67.160753	H	55.183673	5.482698	68.698449	H	54.856243	4.220245	68.839513
H	52.210818	5.303682	68.483987	H	53.849543	4.858270	69.620617	H	53.183984	3.876006	69.132648
H	54.061679	8.026202	67.255569	H	55.575763	7.801153	68.886826	H	55.548891	6.440853	68.533535
H	53.632566	9.118741	68.519163	H	54.217574	8.864864	68.908562	H	54.361033	7.709898	68.402596
H	52.167806	2.187928	62.234633	H	52.583860	1.929728	62.329405	H	52.334972	1.786590	62.367717
H	51.593188	3.100965	63.647048	H	51.563635	3.131235	63.146049	H	51.618799	3.187058	63.185245
H	53.962536	3.776617	63.180120	H	54.035076	3.696054	63.426438	H	54.147882	3.456088	62.846500
H	54.475700	2.100288	63.142590	H	54.312217	2.100268	64.113408	H	54.407344	1.973432	63.753883
H	54.063360	1.794633	65.520292	H	52.782342	2.643417	66.029026	H	53.411173	3.046391	65.801867
H	53.169605	3.298993	65.649127	H	52.496501	4.242607	65.365959	H	53.171670	4.540430	64.912794

H	59.430319	9.335435	66.440862	H	59.613135	10.111140	65.790900	H	59.149329	8.795479	65.417461
H	52.084324	1.409515	63.814368	H	51.852478	1.555734	63.895951	H	51.924740	1.696743	64.089555
H	56.433828	11.236950	69.672731	H	56.992603	11.734932	69.437609	H	56.222036	9.720237	69.176154
H	56.983447	12.549190	68.598054	H	57.006213	13.024971	68.207725	H	56.147872	11.299811	68.372369
H	49.847018	11.244554	66.664828	H	50.058721	10.201166	67.945423	H	49.135937	10.406847	67.472829

Siroheme (Fe²⁺) without SO₃²⁻

S=0			S=1			S=2					
C	51.422358	3.380522	70.997438	C	51.422358	3.380522	70.997438	C	51.422358	3.380522	70.997438
C	51.590579	4.088882	69.650906	C	51.397867	4.150071	69.677266	C	51.824992	4.175627	69.758366
C	52.726085	5.106266	69.698224	C	52.609757	5.066843	69.539141	C	52.977547	5.127906	70.059930
N	52.897838	5.768268	68.398603	N	52.565349	5.782752	68.261560	N	53.406805	5.803335	68.834135
C	53.955593	6.505319	68.080579	C	53.591481	6.442506	67.727164	C	54.577347	6.421642	68.679826
N	54.923384	6.748274	68.954399	N	54.748173	6.554731	68.379038	N	55.417901	6.533995	69.722798
N	54.112924	6.976607	66.802083	N	53.490008	6.944119	66.473313	N	54.941267	6.913397	67.491674
C	55.076348	1.425184	63.280932	C	55.076348	1.425184	63.280932	C	55.076348	1.425184	63.280932
C	56.252289	2.345250	63.604464	C	56.266166	2.298782	63.677717	C	56.381091	2.167521	63.575585
C	56.717252	2.199018	65.058978	C	56.455163	2.345726	65.198184	C	56.682370	2.227038	65.079106
N	57.624919	3.266006	65.492090	N	57.447516	3.333476	65.636300	N	57.718247	3.204796	65.433113
C	57.214948	4.494161	65.833003	C	57.231635	4.651933	65.643136	C	57.509071	4.524833	65.441257
N	55.916743	4.798192	65.775318	N	56.024191	5.153787	65.363241	N	56.293080	5.021303	65.199028
N	58.098814	5.433163	66.208528	N	58.225003	5.519976	65.913318	N	58.518038	5.390241	65.662833
C	60.333112	3.765595	62.506421	C	60.333112	3.765595	62.506421	C	60.333112	3.765595	62.506421
C	60.256756	4.891209	61.442682	C	60.256756	4.891209	61.442682	C	60.256756	4.891209	61.442682
C	60.007232	6.297148	61.987374	C	60.081043	6.295594	62.020575	C	60.107515	6.300340	62.010790
C	61.171049	6.855446	62.801908	C	61.269941	6.772059	62.849375	C	61.349878	6.803647	62.741038
N	61.064195	8.330200	62.939862	N	61.165106	8.226629	63.128425	N	61.236723	8.263354	62.976979
C	55.161658	2.803979	58.893853	C	55.161658	2.803979	58.893853	C	55.161658	2.803979	58.893853
C	55.522484	3.451533	60.237172	C	55.522484	3.451533	60.237172	C	55.522484	3.451533	60.237172
C	55.878926	4.938217	60.167362	C	56.035426	4.886908	60.088352	C	55.965425	4.912349	60.104944
C	56.185425	5.454577	61.565688	C	56.309003	5.497548	61.450568	C	56.264120	5.503897	61.471857
N	56.414060	6.928050	61.602140	N	56.747367	6.923298	61.369543	N	56.594340	6.960238	61.415229
Fe	56.783946	10.314906	63.513839	Fe	57.272019	10.570287	63.346339	Fe	57.094639	10.737805	63.351761
C	60.119866	10.930733	63.636219	C	60.641560	10.949998	63.722408	C	60.549142	10.974845	63.265312
C	56.642736	10.647527	66.863531	C	56.912140	10.921552	66.674399	C	57.243490	10.870484	66.759538
C	53.515638	9.315983	63.465410	C	54.031092	9.527352	63.096092	C	53.860712	9.497270	63.586570
C	56.937131	10.103317	60.098151	C	57.698530	10.208845	59.970298	C	57.128165	9.957654	59.951089
N	58.127526	10.439205	64.939017	N	58.537655	10.621255	64.887337	N	58.648263	10.700275	64.757203
C	59.519374	10.501171	64.777146	C	59.929900	10.571360	64.818910	C	60.012755	10.730627	64.498590
C	60.219225	10.156059	66.083725	C	60.491897	10.180995	66.178880	C	60.778905	10.514244	65.803639
C	60.236575	8.623595	66.297392	C	60.321945	8.657277	66.409225	C	60.778275	9.014066	66.201731
C	61.618027	10.746973	66.270275	C	61.930911	10.610068	66.450180	C	62.198467	11.076813	65.841941
C	62.850880	10.114054	65.584112	C	63.106827	9.872238	65.765138	C	63.352766	10.329939	65.127622
O	62.724934	9.259001	64.620235	O	62.905647	9.012361	64.818633	O	63.124618	9.363668	64.296688
O	63.957671	10.485586	66.018895	O	64.241958	10.161053	66.189703	O	64.500648	10.727080	65.404336
C	59.179024	10.757247	67.049616	C	59.441422	10.897438	67.054988	C	59.782524	11.224744	66.754786
C	57.896390	10.577153	66.275599	C	58.208793	10.792356	66.188148	C	58.464829	10.912416	66.080656
N	55.334258	10.077968	64.889302	N	55.731691	10.441157	64.595215	N	55.777603	10.113432	64.966238
C	55.440985	10.467293	66.199300	C	55.758516	10.789044	65.920047	C	55.987678	10.569600	66.223775
C	54.096029	10.778943	66.826938	C	54.376332	10.988406	66.511299	C	54.682258	10.806788	66.966615
C	53.950189	10.344536	68.286566	C	54.193262	10.324951	67.880731	C	54.699281	10.372695	68.432908
C	53.918606	12.324217	66.712004	C	54.137942	12.522010	66.624072	C	54.400907	12.335365	66.851409
C	52.528868	12.770264	67.225150	C	52.701673	12.828108	67.112761	C	53.051184	12.708405	67.514015
O	52.483266	13.271885	68.384304	O	52.565422	13.135885	68.330573	O	53.108789	13.231151	68.662806
O	51.546949	12.563983	66.448130	O	51.777052	12.706118	66.251743	O	52.001821	12.426643	66.859195
C	53.136146	10.055709	65.861778	C	53.482722	10.368693	65.418339	C	53.686748	10.008817	66.092501
C	53.988400	9.791779	64.649862	C	54.423764	10.092516	64.280564	C	54.420812	9.862490	64.785674
N	55.537237	9.736695	62.100503	N	56.136146	9.858619	61.846220	N	55.768878	9.846674	62.015327
C	54.252934	9.243151	62.269994	C	54.828124	9.438305	61.928382	C	54.480754	9.452062	62.300982

H	60.943057	8.127824	65.626899	H	61.046675	8.078109	65.831575	H	61.493093	8.435090	65.612700
H	59.233608	8.201869	66.148520	H	59.304957	8.341700	66.146322	H	59.776818	8.580552	66.090212
H	60.547868	8.398409	67.326757	H	60.491098	8.432104	67.471397	H	61.076395	8.923455	67.255299
H	61.607892	11.807724	65.977701	H	62.051440	11.677791	66.214205	H	62.202203	12.104741	65.448962
H	61.854534	10.742073	67.343408	H	62.124882	10.524170	67.528762	H	62.516518	11.161428	66.890542
H	59.168284	10.285574	68.040622	H	59.315267	10.452235	68.049822	H	59.836545	10.879432	67.793983
H	54.169392	9.277384	68.424438	H	54.463704	9.260940	67.850942	H	54.991114	9.319851	68.527921
H	52.926072	10.530014	68.631393	H	53.149227	10.409160	68.204563	H	53.701867	10.496720	68.871535
H	54.618498	10.915148	68.943369	H	54.811650	10.806049	68.647906	H	55.389765	10.985928	69.024966
H	54.045322	12.612621	65.660782	H	54.298143	12.977243	65.638096	H	54.388266	12.612918	65.788738
H	54.706720	12.808510	67.301113	H	54.869602	12.940528	67.325865	H	55.217941	12.879135	67.341303
H	52.730424	8.358366	60.893301	H	53.358085	8.650257	60.437989	H	52.807903	8.651167	61.044641
H	54.603206	8.890411	58.983744	H	55.385379	9.106366	58.671604	H	54.587470	8.945553	59.011838
H	59.399320	11.138815	59.073182	H	60.269822	11.122898	59.111764	H	59.663218	10.608279	58.715155
H	61.153164	11.707718	61.080551	H	61.906859	11.619414	61.229001	H	61.534784	11.281393	60.563711
H	54.926506	12.002421	60.926212	H	54.827891	11.919762	61.064150	H	55.020049	11.989905	61.028085
H	54.074559	12.048061	63.309257	H	54.609934	12.470437	63.521556	H	54.282692	12.248423	63.431192
H	54.436259	13.770171	63.405878	H	54.953110	14.170055	63.171621	H	54.445152	14.002766	63.291890
H	52.116973	5.744507	67.748528	H	51.672239	5.825219	67.779901	H	52.762456	5.808367	68.049830
H	58.608208	3.047573	65.605982	H	58.343231	2.998324	65.974038	H	58.623176	2.863289	65.737255
H	60.119559	8.628045	63.213870	H	60.225862	8.480970	63.459001	H	60.349279	8.496056	63.437990
H	55.606906	7.440835	61.183574	H	56.105537	7.496411	60.775391	H	55.880712	7.504542	60.879094
H	53.600327	13.176864	61.111645	H	53.550774	13.127273	61.354876	H	53.564386	13.008946	61.156408
H	55.290133	13.735936	61.028006	H	55.136053	13.632000	60.716667	H	55.160037	13.754231	60.887295
O	56.697191	7.583874	64.328015	O	56.176018	7.590241	64.040226	O	56.120286	7.518288	64.107091
H	57.603616	7.806702	64.612338	H	56.696679	8.412478	64.242029	H	56.408657	8.406986	64.464648
H	56.195289	8.435183	64.510804	H	55.297203	7.993488	63.810780	H	55.176842	7.740162	63.914022
O	57.211493	7.807095	67.726073	O	57.042534	7.912525	67.301732	O	57.594435	7.879639	67.163135
H	57.054591	8.732757	67.385468	H	56.953554	8.866846	67.032246	H	57.521294	8.863302	67.009555
H	57.918603	7.914894	68.388443	H	57.621492	7.955032	68.085164	H	58.229820	7.803775	67.897267
H	55.327556	0.374889	63.478309	H	55.197586	0.398121	63.650731	H	55.100843	0.403726	63.683118
H	52.738427	9.129076	66.304310	H	52.968950	9.461446	65.767028	H	53.488803	9.021087	66.539302
H	52.271143	10.694133	65.633483	H	52.684791	11.071168	65.134828	H	52.732322	10.541681	65.998795
H	59.365223	11.834499	67.192539	H	59.703166	11.960914	67.187112	H	59.946141	12.314891	66.742846

Siroheme (Fe³⁺) without SO₃²⁻

S=1/2			S=3/2			S=5/2					
C	51.422358	3.380522	70.997438	C	51.422358	3.380522	70.997438	C	51.422358	3.380522	70.997438
C	52.009085	4.639696	70.362767	C	52.010841	4.613159	70.319180	C	51.917058	3.458665	69.553207
C	53.524750	4.712678	70.539259	C	53.491843	4.786147	70.650758	C	52.437405	4.855298	69.214662
N	54.041567	5.923054	69.892108	N	54.005586	5.987463	69.988639	N	52.889489	4.910837	67.821613
C	55.233969	6.060698	69.327493	C	55.178531	6.121863	69.386686	C	53.950522	5.566992	67.361667
N	56.186775	5.136912	69.471301	N	56.156500	5.225281	69.531792	N	54.638340	6.411646	68.128636
N	55.475560	7.124477	68.515723	N	55.373773	7.163204	68.532928	N	54.378946	5.342816	66.086791
C	55.076348	1.425184	63.280932	C	55.076348	1.425184	63.280932	C	55.076348	1.425184	63.280932
C	56.042850	2.531370	63.702059	C	55.978965	2.589345	63.690191	C	56.437656	2.031207	63.634455
C	56.310753	2.496572	65.207631	C	56.248529	2.591166	65.195708	C	56.676734	2.073783	65.147444
N	57.300334	3.482170	65.655168	N	57.210780	3.615258	65.621004	N	58.008257	2.570546	65.501887
C	57.035271	4.699608	66.128102	C	56.916539	4.821659	66.103420	C	58.328775	3.795407	65.928086
N	55.819470	5.242512	66.012424	N	55.683333	5.334719	66.005985	N	57.401817	4.751939	66.080472
N	57.994621	5.387841	66.784191	N	57.867858	5.541773	66.737014	N	59.612617	4.089953	66.174815
C	60.333112	3.765595	62.506421	C	60.333112	3.765595	62.506421	C	60.333112	3.765595	62.506421
C	60.256756	4.891209	61.442682	C	60.256756	4.891209	61.442682	C	60.256756	4.891209	61.442682
C	61.362164	5.945117	61.584415	C	60.247692	6.314887	61.999206	C	61.391477	5.909671	61.566517
C	62.763682	5.358453	61.447361	C	61.542751	6.743012	62.688687	C	62.784751	5.309853	61.409170
N	63.801219	6.403383	61.677609	N	61.569553	8.226043	62.819706	N	63.815749	6.317121	61.794655
C	55.161658	2.803979	58.893853	C	55.161658	2.803979	58.893853	C	55.161658	2.803979	58.893853
C	55.522484	3.451533	60.237172	C	55.522484	3.451533	60.237172	C	55.522484	3.451533	60.237172
C	56.042958	4.882654	60.078863	C	56.106934	4.856169	60.056222	C	55.625720	4.974450	60.246960

C	56.361413	5.487322	61.432175	C	56.420194	5.506221	61.390934	C	55.954837	5.403162	61.666781
N	56.913982	6.873826	61.332028	N	57.025534	6.866869	61.225897	N	55.823621	6.866423	61.899132
Fe	57.106579	10.036037	62.903727	Fe	57.468201	10.648801	63.220178	Fe	56.524974	10.060562	63.037322
C	60.383267	9.369065	62.232706	C	60.869227	11.004924	63.168882	C	59.758708	8.927172	62.403792
C	57.875330	10.908579	66.040633	C	57.489124	11.240951	66.518015	C	57.303436	10.174917	66.382599
C	53.890190	9.344568	63.825108	C	54.490344	8.983917	63.504961	C	53.148534	9.759242	63.947534
C	56.307342	9.660786	59.615412	C	57.403596	10.368808	59.843771	C	55.685426	9.431279	59.771885
N	58.807209	10.084179	63.945966	N	58.919259	10.805351	64.593547	N	58.217864	9.471581	64.220258
C	60.067396	9.653583	63.522471	C	60.298919	10.755009	64.375825	C	59.461723	9.099039	63.725014
C	61.016711	9.565526	64.714163	C	61.010503	10.565302	65.704634	C	60.448859	8.911063	64.882055
C	60.832526	8.182139	65.376795	C	60.909912	9.090472	66.167015	C	60.366803	7.438497	65.341485
C	62.495949	9.872600	64.413501	C	62.454970	11.058149	65.761201	C	61.899711	9.368343	64.618947
C	63.210775	8.899895	63.466269	C	63.592788	10.245602	65.096673	C	62.718868	8.516309	63.642995
O	63.333942	7.678490	63.867808	O	63.342631	9.234113	64.326365	O	63.132000	7.376664	64.076946
O	63.621251	9.318113	62.357789	O	64.744978	10.630412	65.359349	O	62.932942	8.954794	62.483865
C	60.378014	10.641199	65.621012	C	60.039493	11.401918	66.575996	C	59.783759	9.804672	65.950296
C	58.935007	10.577705	65.205377	C	58.725058	11.151062	65.887071	C	58.342833	9.821625	65.521662
N	56.093456	10.038802	64.621078	N	56.208620	10.220153	64.717763	N	55.399314	9.832637	64.897199
C	56.548303	10.609316	65.781205	C	56.312880	10.759101	65.967718	C	55.943235	10.207292	66.088802
C	55.416358	10.869385	66.758585	C	54.998176	10.675996	66.714564	C	54.888446	10.716032	67.048983
C	55.776928	10.733301	68.236379	C	55.122130	10.540657	68.231301	C	55.103779	10.319346	68.507896
C	54.903672	12.311320	66.472875	C	54.196508	11.966371	66.371343	C	54.904108	12.265475	66.874991
C	53.714010	12.686885	67.397246	C	52.807629	11.957880	67.073584	C	53.783433	12.933055	67.715885
O	53.930015	13.581034	68.257603	O	52.642689	12.790714	68.002008	O	54.132143	13.443348	68.814616
O	52.635849	12.043919	67.215155	O	51.976712	11.095421	66.655837	O	52.614290	12.879202	67.232670
C	54.387907	9.836979	66.259428	C	54.364441	9.462704	65.998763	C	53.610081	10.113291	66.428523
C	54.755153	9.695822	64.814979	C	55.011795	9.519143	64.646935	C	54.008696	9.882620	65.000089
N	55.450324	9.560573	61.927782	N	56.216760	9.805766	61.933320	N	54.760938	9.594724	62.067335
C	54.197607	9.331129	62.453939	C	55.026267	9.169514	62.211235	C	53.482677	9.631217	62.578793
C	53.237501	9.142849	61.409895	C	54.387088	8.768350	60.999910	C	52.529065	9.561878	61.514746
C	53.904250	9.291010	60.218071	C	55.185367	9.206690	59.957497	C	53.237691	9.494345	60.335078
C	55.276895	9.543641	61.534814	C	56.321263	9.843847	60.540046	C	54.626702	9.512394	60.673420
N	58.133655	9.633050	61.261502	N	58.837170	10.734115	61.804545	N	57.521781	9.252510	61.401920
C	57.650952	9.676593	59.947503	C	58.578127	10.794266	60.431463	C	57.035076	9.321412	60.090350
C	58.734659	9.534345	59.026023	C	59.754354	11.220409	59.738418	C	58.121359	9.154531	59.176343
C	59.878033	9.374491	59.773846	C	60.740932	11.386285	60.682007	C	59.262709	8.981365	59.929081
C	59.492874	9.456104	61.149089	C	60.158238	11.081371	61.952420	C	58.878809	9.050636	61.306209
C	54.634215	12.941636	61.407585	C	54.634215	12.941636	61.407585	C	54.634215	12.941636	61.407585
C	55.305075	12.714181	62.757194	C	55.057210	12.836374	62.867590	C	55.093336	12.891779	62.858598
S	57.031891	12.124365	62.622111	S	56.877759	12.848952	63.073648	S	56.818881	12.268847	63.014196
H	55.561337	6.035848	66.600472	H	55.409847	6.083498	66.646935	H	57.615646	5.597465	66.618848
H	50.335009	3.349458	70.858804	H	50.361833	3.267345	70.744014	H	51.065322	2.369762	71.228516
H	51.624296	3.347219	72.076065	H	51.500146	3.453905	72.090685	H	50.592311	4.078873	71.171145
H	51.845580	2.472689	70.545898	H	51.942548	2.465346	70.682364	H	52.225262	3.624785	71.706649
H	51.776951	4.666928	69.287764	H	51.898697	4.540449	69.227725	H	52.723681	2.729825	69.384596
H	51.554903	5.534539	70.814243	H	51.466877	5.514465	70.639640	H	51.099283	3.201981	68.862102
H	53.793542	4.714970	71.606069	H	53.644369	4.866045	71.736342	H	51.657536	5.613071	69.380931
H	53.998105	3.839868	70.067859	H	54.060402	3.919240	70.288796	H	53.287880	5.095091	69.866727
H	57.036539	5.186967	68.915908	H	56.992636	5.284871	68.957689	H	55.567914	6.761718	67.856185
H	56.079629	4.369345	70.122306	H	56.098313	4.490644	70.225119	H	54.314624	6.621177	69.064807
H	56.435734	7.486939	68.437042	H	56.320932	7.562544	68.445883	H	54.870223	6.115455	65.609157
H	54.768571	7.855419	68.517940	H	54.644536	7.872371	68.532679	H	53.737670	4.830245	65.488729
H	54.912253	1.439249	62.198134	H	54.900482	1.427880	62.200168	H	54.962933	1.329426	62.195932
H	54.100191	1.543721	63.770660	H	54.099964	1.484665	63.779938	H	54.250061	2.045546	63.655920
H	55.635274	3.514650	63.425263	H	55.518951	3.545270	63.400427	H	56.527190	3.049159	63.228188
H	57.000877	2.422338	63.172237	H	56.942144	2.525139	63.163256	H	57.240557	1.437968	63.172253
H	56.697868	1.512396	65.498920	H	56.665976	1.625364	65.505133	H	56.586804	1.065252	65.571835
H	55.383901	2.648925	65.779207	H	55.319174	2.725989	65.766241	H	55.916706	2.684108	65.653629

H	55.073928	4.747440	65.538976	H	54.937876	4.793305	65.584759	H	56.410835	4.522761	66.020978
H	58.921078	4.976632	66.834442	H	58.810555	5.166068	66.757341	H	60.330457	3.377614	66.142587
H	57.970943	6.417095	66.810294	H	57.810026	6.567343	66.755316	H	59.880128	5.009984	66.501270
H	59.450409	3.115375	62.448608	H	60.299728	2.780794	62.026623	H	59.437475	3.131868	62.467651
H	60.380906	4.192851	63.518004	H	59.486325	3.835103	63.205530	H	60.403973	4.195026	63.515356
H	61.215529	3.130929	62.362920	H	61.259742	3.824822	63.091442	H	61.201575	3.114439	62.351053
H	60.280783	4.451415	60.434734	H	61.098982	4.789039	60.743041	H	60.248070	4.448615	60.435643
H	59.288400	5.403659	61.536399	H	59.350615	4.740343	60.835647	H	59.307284	5.435712	61.552352
H	61.276259	6.435803	62.565105	H	59.417999	6.441330	62.715051	H	61.330459	6.384887	62.554599
H	61.218538	6.729298	60.826493	H	60.074116	7.012867	61.163337	H	61.255552	6.708646	60.824630
H	62.913444	4.915006	60.454799	H	62.425202	6.448270	62.110885	H	62.970093	4.981283	60.379731
H	62.939739	4.580302	62.197731	H	61.636783	6.318799	63.693574	H	62.929424	4.451606	62.073824
H	64.744118	6.008357	61.629741	H	61.722220	8.663675	61.904703	H	64.766178	5.953658	61.694533
H	63.663264	6.925592	62.680620	H	62.335870	8.679979	63.539820	H	63.634275	6.683778	62.829882
H	54.793986	1.780414	59.037314	H	54.746703	1.799071	59.039463	H	55.095071	1.714211	58.998798
H	56.036360	2.759073	58.231139	H	56.047500	2.713742	58.250915	H	55.917463	3.024239	58.127774
H	54.377736	3.376153	58.380168	H	54.414400	3.403990	58.357597	H	54.193260	3.169070	58.525794
H	56.287194	2.844875	60.744697	H	56.252731	2.822621	60.767035	H	56.476383	3.028959	60.591841
H	54.638275	3.460719	60.892327	H	54.627856	3.509939	60.874925	H	54.765262	3.161602	60.980889
H	55.292602	5.502607	59.565435	H	55.396142	5.487688	59.502058	H	54.667342	5.419974	59.938337
H	56.947997	4.883009	59.451551	H	57.024472	4.798566	59.449819	H	56.395214	5.330004	59.546783
H	57.111498	4.893282	61.968315	H	57.132487	4.913296	61.976940	H	56.977986	5.124515	61.946546
H	55.467566	5.559921	62.062280	H	55.513831	5.647583	61.991573	H	55.266044	4.921567	62.371563
H	57.752049	6.919641	60.739991	H	57.896145	6.829044	60.685340	H	56.585825	7.444254	61.492433
H	57.166126	7.216607	62.294500	H	57.227403	7.268892	62.176741	H	55.836692	7.057435	62.932897
H	61.414832	9.129231	61.992181	H	61.951656	11.097153	63.115697	H	60.799054	8.733447	62.153506
H	58.112453	11.387258	66.989250	H	57.460215	11.654689	67.523364	H	57.596953	10.530523	67.369595
H	52.860415	9.131663	64.105455	H	53.537224	8.463406	63.577605	H	52.085044	9.817641	64.173932
H	56.044818	9.652859	58.558645	H	57.337717	10.399029	58.757461	H	55.425286	9.414969	58.714172
H	61.125215	7.378279	64.696096	H	61.575286	8.446007	65.587351	H	60.680006	6.754530	64.547349
H	59.787322	8.041264	65.686598	H	59.881928	8.715166	66.086319	H	59.331261	7.202638	65.628906
H	61.458969	8.107351	66.275058	H	61.221685	9.024088	67.218190	H	61.018156	7.277931	66.210705
H	62.574192	10.880833	63.990663	H	62.516809	12.077078	65.351680	H	61.878239	10.400930	64.250732
H	63.034402	9.860882	65.372903	H	62.746215	11.149140	66.817058	H	62.420466	9.357941	65.587117
H	60.531565	10.461658	66.691513	H	60.035109	11.122562	67.635615	H	59.929803	9.447258	66.976407
H	56.269603	9.778708	68.455686	H	55.849908	9.775076	68.524628	H	55.175414	9.228363	68.610497
H	54.866812	10.805076	68.844662	H	54.143737	10.292699	68.662470	H	54.261153	10.669643	69.115390
H	56.443659	11.540998	68.562360	H	55.434995	11.487032	68.688414	H	56.010722	10.774671	68.923870
H	54.575549	12.377477	65.427311	H	54.046580	12.023153	65.286510	H	54.755290	12.507106	65.813550
H	55.729449	13.016709	66.625300	H	54.771458	12.841816	66.693049	H	55.883925	12.645947	67.188199
H	52.183241	8.941056	61.570674	H	53.432639	8.254897	60.942195	H	51.451910	9.576901	61.646796
H	53.507759	9.222021	59.209897	H	55.008110	9.110405	58.890935	H	52.848505	9.445222	59.322815
H	58.629186	9.527764	57.945676	H	59.824170	11.351480	58.663141	H	58.028574	9.161342	58.094758
H	60.896792	9.236244	59.425186	H	61.773476	11.685252	60.531891	H	60.277603	8.830918	59.574537
H	54.531591	12.000268	60.855693	H	55.003873	12.086278	60.829789	H	54.638291	11.946349	60.954079
H	54.741416	11.995565	63.362754	H	54.664973	11.916250	63.315549	H	54.437174	12.253657	63.463385
H	55.371841	13.649851	63.329915	H	54.676245	13.682761	63.452997	H	55.098725	13.889811	63.313263
H	53.407400	6.715798	69.834890	H	53.359100	6.769104	69.912952	H	52.341338	4.384341	67.147336
H	58.271056	3.186378	65.672071	H	58.189662	3.346505	65.634286	H	58.781653	1.933286	65.338346
H	63.752530	7.160941	60.987115	H	60.662678	8.581391	63.142614	H	63.731729	7.183562	61.246222
H	56.233430	7.546056	60.936128	H	56.374077	7.508063	60.728997	H	54.944953	7.244683	61.523789
H	53.631364	13.363920	61.559800	H	53.537451	12.957855	61.338647	H	53.610871	13.339533	61.359066
H	55.211539	13.641670	60.790582	H	55.022001	13.858979	60.947778	H	55.284944	13.593809	60.812124
O	57.450390	7.415877	64.003139	O	57.302368	7.432274	63.960672	O	56.005328	7.194160	64.639763
H	58.327535	7.835070	64.115823	H	57.727056	8.296878	64.144379	H	56.969210	7.134689	64.775913
H	56.833801	8.081123	64.385872	H	56.352500	7.643332	64.105777	H	55.796111	8.176204	64.745981
O	58.013139	8.149300	67.532726	O	57.843184	8.305867	67.611279	O	57.308472	7.304272	67.527500
H	57.916700	9.008587	67.052716	H	57.715567	9.218096	67.254186	H	57.317552	8.229308	67.173628

H	58.773152	8.284841	68.127112	H	58.609142	8.382745	68.208818	H	57.785383	7.359358	68.376068
H	55.470625	0.435454	63.548204	H	55.532969	0.462213	63.545293	H	54.968958	0.422673	63.717246
H	54.531936	8.866812	66.762556	H	54.645057	8.522352	66.499209	H	53.367231	9.150784	66.909239
H	53.361298	10.182531	66.425040	H	53.271453	9.545486	65.969191	H	52.751865	10.787238	66.534241
H	60.781314	11.637928	65.380119	H	60.282587	12.474717	66.503911	H	60.174663	10.833311	65.896483

Siroheme (Fe²⁺) without NO₂⁻

S=0			S=1			S=2					
C	50.353397	-52.121132	49.522288	C	50.353397	-52.121132	49.522288	C	50.353397	-52.121132	49.522288
C	50.586451	-50.763991	50.185071	C	50.191970	-50.603022	49.582184	C	50.407619	-50.613648	49.740255
C	52.073921	-50.444107	50.271897	C	51.445832	-49.898247	49.077958	C	51.524465	-49.981119	48.919636
N	52.289015	-49.124490	50.869378	N	51.272764	-48.444854	49.111468	N	51.509014	-48.528320	49.089492
C	53.455874	-48.480718	50.857417	C	52.080105	-47.580581	48.495159	C	52.460520	-47.697467	48.679888
N	54.526429	-49.050492	50.283610	N	53.152914	-48.038650	47.827935	N	53.480381	-48.140910	47.913405
N	53.560990	-47.260942	51.404363	N	51.816802	-46.270927	48.505831	N	52.431022	-46.401618	49.015384
C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410
C	53.703505	-47.148801	42.844276	C	53.688451	-47.103964	42.901048	C	53.676672	-47.063731	42.937345
C	53.897909	-47.787584	44.223905	C	53.895619	-48.100751	44.045848	C	53.810728	-46.884419	44.453382
N	55.298837	-48.081479	44.531700	N	55.272231	-48.180604	44.541571	N	55.199360	-47.112786	44.858710
C	56.148159	-47.311340	45.220892	C	55.804796	-47.393209	45.484610	C	55.986117	-46.392566	45.666401
N	55.758047	-46.208624	45.869976	N	55.046690	-46.400769	46.026431	N	55.549174	-45.239767	46.241290
N	57.452091	-47.625192	45.249837	N	57.045735	-47.583737	45.922754	N	57.238087	-46.781518	45.887414
C	57.646397	-45.007662	42.604348	C	57.646397	-45.007662	42.604348	C	57.646397	-45.007662	42.604348
C	57.606397	-43.479422	42.863688	C	57.606397	-43.479422	42.863688	C	57.606397	-43.479422	42.863688
C	57.939624	-43.117970	44.316241	C	57.693263	-43.120937	44.349542	C	58.201658	-43.111471	44.230161
C	59.416453	-43.351550	44.619426	C	59.026868	-43.520245	44.969282	C	59.716886	-43.291270	44.247626
N	59.664557	-43.345161	46.090669	N	58.984822	-43.342899	46.452546	N	60.250257	-43.186205	45.641240
C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430
C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930
C	53.154706	-42.444454	43.121748	C	53.232217	-42.450474	43.074418	C	53.445816	-42.468234	42.894720
C	53.777181	-43.233895	44.264497	C	53.756892	-43.245469	44.258392	C	54.130191	-43.247715	44.001268
N	54.264672	-42.362832	45.378851	N	54.386342	-42.402625	45.322880	N	55.027226	-42.402317	44.832220
Fe	54.937796	-41.864098	48.972236	Fe	54.887032	-42.150718	49.517931	Fe	54.617980	-41.489044	48.155762
C	58.109933	-43.050132	49.305287	C	57.810980	-43.827099	49.903675	C	57.541022	-43.087274	48.803243
C	53.951362	-43.802976	51.525331	C	53.532482	-44.070652	51.915159	C	52.991833	-43.529658	50.297069
C	51.712594	-41.417959	47.986674	C	51.847437	-41.562015	48.160203	C	51.542336	-40.623486	46.709381
C	56.005972	-39.469437	46.787832	C	56.395409	-39.965031	47.401737	C	56.214868	-39.495831	45.756257
N	55.790079	-43.286350	50.014304	N	55.471651	-43.722770	50.512511	N	55.141805	-43.245365	49.172945
C	57.108381	-43.750798	49.905041	C	56.640980	-44.435294	50.243066	C	56.436829	-43.710824	49.333553
C	57.276470	-45.023384	50.728733	C	56.392580	-45.872524	50.658340	C	56.427417	-44.929240	50.268142
C	56.630074	-46.254841	50.048977	C	55.312225	-46.559654	49.779830	C	56.057073	-46.192156	49.455305
C	58.704414	-45.341673	51.165115	C	57.641186	-46.745470	50.666094	C	57.705491	-45.145870	51.097758
C	59.736343	-45.902404	50.155836	C	58.138929	-47.168429	49.260550	C	59.011285	-45.328243	50.294756
O	59.444174	-46.067224	48.905645	O	57.875503	-46.407328	48.233426	O	59.002294	-46.211062	49.348540
O	60.847700	-46.196148	50.635289	O	58.778125	-48.228866	49.163513	O	59.988430	-44.603861	50.577858
C	56.343927	-44.616863	51.894788	C	55.668248	-45.534800	51.997567	C	55.188405	-44.565816	51.122501
C	55.275863	-43.853958	51.152216	C	54.835013	-44.355088	51.516438	C	54.362271	-43.749287	50.155601
N	53.167870	-42.501314	49.624004	N	53.034380	-42.598994	50.031822	N	52.575831	-42.054012	48.395427
C	52.948325	-43.264790	50.734141	C	52.666090	-43.328847	51.135352	C	52.156508	-42.796453	49.461540
C	51.472510	-43.471330	51.035058	C	51.160304	-43.334450	51.344558	C	50.643871	-42.753508	49.642515
C	51.119479	-44.910525	51.423762	C	50.611327	-44.694357	51.787328	C	50.022665	-44.154098	49.727101
C	51.071511	-42.480608	52.162329	C	50.810154	-42.236800	52.387382	C	50.330343	-41.941958	50.926921
C	49.593802	-42.669522	52.580140	C	49.288024	-42.180757	52.670674	C	48.805380	-41.880044	51.191167
O	49.387165	-43.281917	53.667230	O	48.898496	-42.635018	53.782738	O	48.354271	-42.651520	52.086063
O	48.717690	-42.225216	51.779537	O	48.561272	-41.701800	51.747501	O	48.140214	-41.085308	50.462656
C	50.841535	-43.069959	49.689990	C	50.669188	-42.921419	49.943060	C	50.191413	-42.009584	48.363427
C	51.925713	-42.269913	49.027318	C	51.882115	-42.300824	49.313716	C	51.471085	-41.513925	47.747734
N	54.045313	-40.666991	47.690891	N	54.255423	-41.045799	47.999983	N	54.004366	-40.415942	46.394679
C	52.698756	-40.622378	47.379686	C	52.953597	-40.884929	47.589853	C	52.698255	-40.046031	46.129956

C	52.448717	-39.650050	46.355404	C	52.884034	-39.913903	46.542107	C	52.683410	-38.926253	45.240412
C	53.653935	-39.052639	46.062423	C	54.170948	-39.424068	46.361581	C	53.995619	-38.580258	44.990910
C	54.642904	-39.691023	46.878631	C	55.017580	-40.130294	47.267305	C	54.821764	-39.491943	45.716526
N	56.698648	-41.368165	48.193355	N	56.749379	-41.861305	48.919200	N	56.525922	-41.428508	47.254447
C	56.976136	-40.254950	47.393123	C	57.212673	-40.760892	48.187004	C	57.020503	-40.368351	46.495832
C	58.386448	-40.066554	47.274533	C	58.643847	-40.689565	48.281595	C	58.436782	-40.264573	46.685914
C	58.985310	-41.073674	48.008671	C	59.048328	-41.772634	49.040403	C	58.793464	-41.257213	47.583489
C	57.928563	-41.866920	48.561856	C	57.872254	-42.505343	49.397779	C	57.594627	-41.974904	47.916788
C	52.840247	-39.229452	50.941678	C	52.840247	-39.229452	50.941678	C	52.840247	-39.229452	50.941678
C	53.944267	-40.057244	51.586594	C	53.763876	-39.992781	51.884559	C	54.097768	-40.067913	51.116482
S	55.403497	-40.351964	50.530191	S	55.317880	-40.514626	51.070487	S	55.214528	-39.917904	49.666243
H	56.479429	-45.748396	46.460508	H	55.543257	-45.629177	46.518387	H	56.091231	-44.916802	47.044708
H	49.282124	-52.345202	49.463687	H	49.451196	-52.622199	49.892483	H	49.548846	-52.571264	50.115828
H	50.835110	-52.928566	50.090058	H	51.199961	-52.455467	50.137476	H	51.296596	-52.600013	49.818891
H	50.757821	-52.137498	48.501093	H	50.527773	-52.460712	48.491967	H	50.168071	-52.363259	48.466867
H	50.081991	-49.970602	49.614428	H	49.334215	-50.287518	48.970463	H	49.448901	-50.157736	49.450388
H	50.155716	-50.759024	51.197047	H	49.989240	-50.284490	50.615492	H	50.568228	-50.384016	50.803334
H	52.590696	-51.213193	50.868069	H	52.313122	-50.186817	49.693514	H	52.500624	-50.367818	49.248710
H	52.510927	-50.443193	49.262533	H	51.646930	-50.201690	48.039657	H	51.395283	-50.231293	47.854823
H	55.422955	-48.578957	50.321277	H	53.820687	-47.379390	47.424888	H	54.368463	-47.658209	48.010561
H	54.540632	-50.049024	50.116935	H	53.501825	-48.967242	48.031802	H	53.546996	-49.134202	47.722258
H	54.420909	-46.734400	51.293933	H	52.450919	-45.582539	48.078689	H	52.795035	-45.701826	48.357109
H	52.726769	-46.708883	51.585636	H	50.946834	-45.932104	48.898084	H	51.687655	-46.067783	49.620785
H	52.104145	-46.580694	41.481174	H	52.086811	-46.373354	41.619506	H	52.183571	-47.183688	41.366395
H	51.647460	-46.492965	43.192173	H	51.567067	-46.747564	43.274709	H	51.711724	-46.133352	42.713561
H	54.160851	-46.148104	42.840643	H	54.010918	-46.099129	43.217011	H	54.249951	-46.271305	42.433687
H	54.252640	-47.745522	42.101776	H	54.341149	-47.383970	42.062679	H	54.155328	-48.015111	42.659270
H	53.355172	-48.740400	44.277026	H	53.628243	-49.109624	43.711709	H	53.158836	-47.591411	44.986668
H	53.478381	-47.152671	45.014253	H	53.226105	-47.874100	44.888779	H	53.510009	-45.875258	44.752645
H	54.789321	-46.064358	46.130425	H	54.233339	-46.107809	45.495515	H	54.537730	-45.079712	46.359514
H	57.829204	-48.383701	44.697303	H	57.545752	-48.406613	45.602617	H	57.601768	-47.600908	45.414653
H	58.076084	-47.116716	45.865970	H	57.414011	-47.132520	46.807918	H	57.917498	-46.152190	46.383112
H	57.392846	-45.230929	41.561173	H	57.479043	-45.221852	41.542380	H	57.202132	-45.249003	41.631488
H	56.921126	-45.522779	43.248443	H	56.862104	-45.521915	43.179528	H	57.083318	-45.546154	43.376735
H	58.636607	-45.435377	42.803684	H	58.610808	-45.448500	42.883408	H	58.671494	-45.395801	42.605564
H	58.299840	-42.964112	42.183253	H	58.420586	-42.986417	42.313873	H	58.152337	-42.950110	42.069907
H	56.604349	-43.099455	42.618535	H	56.671609	-43.068179	42.457205	H	56.569753	-43.128352	42.789434
H	57.330794	-43.740241	44.991662	H	56.899761	-43.657877	44.894827	H	57.755959	-43.755545	45.005997
H	57.691149	-42.066870	44.526268	H	57.538584	-42.039557	44.492354	H	57.971504	-42.070106	44.501197
H	60.044433	-42.581913	44.159481	H	59.855902	-42.926681	44.571661	H	60.205878	-42.523653	43.639281
H	59.747218	-44.328860	44.254048	H	59.240498	-44.578756	44.791962	H	60.015729	-44.273831	43.870555
H	59.411900	-42.432224	46.531905	H	58.969169	-42.350949	46.763322	H	59.891897	-42.328218	46.109004
H	60.645929	-43.536417	46.312571	H	59.793410	-43.775201	46.909555	H	61.273886	-43.161683	45.656998
H	51.416744	-43.512353	40.245855	H	51.365991	-43.509229	40.276946	H	51.191694	-43.468287	40.392959
H	52.543359	-42.142481	40.333111	H	52.554730	-42.190788	40.299424	H	52.575439	-42.372966	40.194003
H	51.018912	-42.097942	41.243016	H	51.058011	-42.053189	41.245701	H	51.215632	-41.906055	41.236450
H	53.315366	-44.093052	41.743914	H	53.269612	-44.142592	41.744990	H	53.123943	-44.270350	41.759240
H	51.803567	-44.045936	42.643564	H	51.785996	-43.991315	42.681088	H	51.771257	-43.817691	42.798743
H	52.383398	-41.770543	43.525180	H	52.524607	-41.688905	43.435270	H	52.868357	-41.635519	43.323705
H	53.914865	-41.813694	42.636708	H	54.052920	-41.921431	42.568050	H	54.200794	-42.029672	42.223783
H	54.629126	-43.839085	43.929325	H	54.510343	-43.980440	43.944955	H	54.731681	-44.065930	43.585794
H	53.037186	-43.907910	44.712261	H	52.936822	-43.783583	44.746978	H	53.393308	-43.674932	44.688891
H	55.084912	-41.799215	45.127699	H	55.358741	-42.155124	45.112613	H	55.671698	-41.842654	44.261948
H	54.493327	-42.939384	46.227343	H	54.345945	-42.915839	46.230296	H	55.601211	-42.958720	45.481499
H	59.125300	-43.433698	49.383510	H	58.730170	-44.408879	49.895603	H	58.509227	-43.391302	49.200585
H	53.665397	-44.289221	52.456561	H	53.125199	-44.614852	52.763527	H	52.518612	-44.013070	51.150853
H	50.691234	-41.305809	47.625079	H	50.872644	-41.384326	47.708258	H	50.591923	-40.245478	46.332990
H	56.342279	-38.650085	46.153014	H	56.864868	-39.172167	46.820320	H	56.721352	-38.704372	45.204420

H	57.190667	-46.594269	49.176611	H	55.652824	-46.691416	48.751622	H	56.846936	-46.456686	48.747496
H	55.598720	-46.037942	49.737141	H	54.376597	-45.989524	49.780457	H	55.104926	-46.010200	48.938235
H	56.633518	-47.074045	50.785123	H	55.100274	-47.551418	50.200772	H	55.919667	-47.041838	50.137235
H	59.160817	-44.448951	51.616251	H	58.473718	-46.240313	51.178858	H	57.844699	-44.299561	51.780785
H	58.662943	-46.087624	51.972769	H	57.456558	-47.674406	51.220214	H	57.563091	-46.048688	51.711166
H	51.426900	-45.598655	50.622102	H	51.000542	-45.499112	51.148205	H	50.242206	-44.730909	48.817676
H	50.035836	-45.013599	51.555934	H	49.515962	-44.691677	51.731335	H	48.932550	-44.075138	49.817142
H	51.581534	-45.195842	52.379667	H	50.884872	-44.923002	52.824303	H	50.374348	-44.699314	50.614938
H	51.225892	-41.456975	51.795655	H	51.138540	-41.264584	51.997198	H	50.725645	-40.926578	50.806076
H	51.722706	-42.645847	53.029870	H	51.351467	-42.445568	53.318458	H	50.832735	-42.414744	51.780080
H	51.469947	-39.431662	45.938313	H	51.971633	-39.592619	46.048497	H	51.785973	-38.436320	44.874595
H	53.859623	-38.269631	45.338676	H	54.500265	-38.650107	45.674799	H	54.362806	-37.765591	44.373687
H	58.861718	-39.262832	46.720390	H	59.258697	-39.911891	47.838282	H	59.077332	-39.512503	46.234167
H	60.042958	-41.212414	48.220446	H	60.061813	-42.053146	49.313725	H	59.764216	-41.422489	48.045747
H	52.438807	-39.739099	50.057528	H	52.542316	-39.855849	50.094507	H	52.293956	-39.538514	50.040712
H	53.561721	-41.021078	51.945280	H	53.264366	-40.881375	52.287339	H	53.846483	-41.127032	51.257681
H	54.356561	-39.535831	52.464328	H	54.050415	-39.364691	52.739346	H	54.664921	-39.742808	51.998806
H	51.523941	-48.709474	51.392878	H	50.509218	-48.070913	49.666667	H	50.674246	-48.116612	49.497597
H	55.700467	-48.889846	44.066773	H	55.854329	-48.933815	44.190483	H	55.633103	-47.936871	44.450708
H	59.052631	-44.086854	46.556048	H	58.101332	-43.793687	46.830908	H	59.915699	-44.002065	46.234276
H	53.532711	-41.689011	45.684064	H	53.869635	-41.503424	45.475213	H	54.491924	-41.690444	45.456272
H	52.012380	-39.063432	51.647142	H	51.929254	-38.904099	51.466167	H	52.171100	-39.332399	51.808049
H	53.224386	-38.251995	50.621730	H	53.343423	-38.339483	50.540406	H	53.094369	-38.167367	50.827213
O	54.383698	-44.182363	47.521684	O	53.421623	-44.130812	47.415467	O	52.933842	-44.446743	46.928219
H	54.955889	-44.032489	48.322344	H	53.995385	-43.894543	48.192911	H	52.939141	-43.564102	47.399105
H	53.493068	-44.011462	47.892323	H	52.685033	-43.475682	47.542264	H	52.052157	-44.505445	46.519243
O	57.910186	-45.088291	47.234887	O	56.603676	-44.451277	47.257407	O	58.957119	-45.072653	47.129126
H	57.501537	-44.372232	47.774015	H	56.299629	-43.730087	47.861895	H	58.385629	-44.358553	47.505632
H	58.519580	-45.538314	48.010331	H	57.061462	-45.153649	47.867636	H	59.161361	-45.601167	48.031111
H	51.782450	-48.070889	42.390114	H	51.892837	-48.061324	42.124932	H	51.663792	-47.897146	42.906252
H	56.873078	-43.936367	52.581629	H	56.389133	-45.209578	52.764822	H	55.474754	-43.923283	51.971009
H	55.965814	-45.464123	52.481934	H	55.059665	-46.354199	52.396431	H	54.656795	-45.438667	51.518811
H	50.611687	-43.967194	49.091201	H	50.341232	-43.801864	49.365949	H	49.668343	-42.690072	47.673747
H	49.909185	-42.511719	49.832966	H	49.812209	-42.238933	50.008733	H	49.487517	-41.203186	48.606473

Siroheme (Fe³⁺) without NO₂⁻

S=1/2			S=3/2			S=5/2					
C	50.353397	-52.121132	49.522288	C	50.353397	-52.121132	49.522288	C	50.353397	-52.121132	49.522288
C	50.454781	-50.611631	49.734789	C	50.491166	-50.626150	49.798373	C	50.664487	-50.757622	50.136012
C	51.779271	-50.069009	49.211069	C	51.949269	-50.192454	49.724647	C	52.167966	-50.540361	50.269024
N	51.877033	-48.624472	49.452553	N	52.065937	-48.746936	49.947401	N	52.446185	-49.217861	50.834646
C	52.831722	-47.849174	48.966172	C	53.208540	-48.083482	49.924105	C	53.634752	-48.618421	50.803571
N	53.840845	-48.356413	48.259534	N	54.363287	-48.705190	49.706053	N	54.687363	-49.239263	50.250075
N	52.767427	-46.485812	49.119610	N	53.198909	-46.711543	50.025693	N	53.780618	-47.383847	51.308653
C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410
C	53.683510	-47.163422	42.904752	C	53.699291	-47.053772	42.865118	C	53.705524	-47.197286	42.820813
C	53.835254	-48.005594	44.174454	C	53.907951	-47.622301	44.271998	C	53.918277	-47.396292	44.325695
N	55.234645	-48.213238	44.555838	N	55.323259	-47.769112	44.615416	N	55.293838	-47.794272	44.629918
C	55.945323	-47.455640	45.394353	C	56.045111	-46.982777	45.419375	C	56.197659	-47.129296	45.353779
N	55.375569	-46.502710	46.157262	N	55.470329	-46.009659	46.155786	N	55.900936	-46.021127	46.046873
N	57.263664	-47.662106	45.523242	N	57.370580	-47.130403	45.502905	N	57.471225	-47.553816	45.364499
C	57.646397	-45.007662	42.604348	C	57.646397	-45.007662	42.604348	C	57.646397	-45.007662	42.604348
C	57.606397	-43.479422	42.863688	C	57.606397	-43.479422	42.863688	C	57.606397	-43.479422	42.863688
C	57.906450	-43.113118	44.323758	C	58.110346	-43.114706	44.264852	C	58.009662	-43.110955	44.298678
C	59.329291	-43.478369	44.734768	C	59.606979	-43.374309	44.408286	C	59.492309	-43.369059	44.549622
N	59.480420	-43.401777	46.221270	N	60.014447	-43.340038	45.847708	N	59.815468	-43.265801	46.005831
C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430
C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930
C	53.346881	-42.390555	42.910653	C	52.335607	-42.765965	43.487128	C	53.355289	-42.474809	42.995373

C	53.918339	-42.957014	44.199317	C	52.919974	-43.707483	44.532666	C	53.850959	-43.260023	44.197452
N	54.725871	-41.902100	44.903372	N	52.755389	-43.216482	45.937280	N	54.507533	-42.407967	45.242103
Fe	54.986149	-41.903946	49.050763	Fe	54.852757	-41.695951	48.479715	Fe	55.179188	-41.643499	49.363191
C	58.016828	-43.340333	49.632094	C	57.993160	-42.867263	49.122967	C	58.357552	-43.046526	49.496173
C	53.595991	-43.960076	51.311692	C	53.650220	-43.703348	50.932695	C	54.163140	-43.974172	51.626617
C	51.937598	-41.275662	47.675842	C	51.637355	-40.844478	47.599138	C	51.907715	-41.543720	48.102228
C	56.454981	-39.567101	47.034105	C	56.059342	-39.806445	45.874190	C	56.204497	-39.599071	46.820188
N	55.620929	-43.463544	50.056864	N	55.633385	-43.184875	49.612769	N	56.054320	-43.365267	50.219223
C	56.904229	-44.016638	50.020029	C	56.969727	-43.579564	49.664105	C	57.368892	-43.784364	50.087886
C	56.859221	-45.403967	50.649982	C	57.112778	-44.817250	50.546498	C	57.541794	-45.104778	50.837830
C	56.156583	-46.427462	49.718822	C	56.690148	-46.101389	49.790722	C	56.917222	-46.290392	50.057402
C	58.206920	-45.951084	51.100118	C	58.473385	-45.002902	51.214905	C	58.967463	-45.436542	51.264224
C	59.242818	-46.361739	50.021560	C	59.703498	-45.474418	50.403121	C	60.008244	-45.887690	50.207475
O	58.997568	-46.203899	48.754854	O	59.635897	-45.668355	49.126233	O	59.719132	-45.933693	48.945171
O	60.301534	-46.851628	50.448488	O	60.738469	-45.659761	51.067872	O	61.121032	-46.208890	50.658804
C	55.857735	-45.058499	51.779265	C	55.983476	-44.489107	51.544343	C	56.568703	-44.795834	52.007514
C	54.943970	-44.104668	51.048435	C	55.001682	-43.765432	50.661728	C	55.507138	-44.002910	51.283036
N	53.119118	-42.479340	49.443042	N	52.979110	-42.250468	49.092185	N	53.331114	-42.672791	49.738525
C	52.725248	-43.268038	50.488663	C	52.707912	-43.048100	50.161790	C	53.142065	-43.420573	50.859935
C	51.214380	-43.296370	50.670571	C	51.232257	-43.103807	50.514206	C	51.670354	-43.581557	51.198088
C	50.617677	-44.655106	51.052188	C	50.696321	-44.539502	50.595099	C	51.278530	-45.019457	51.553307
C	50.892636	-42.245589	51.775055	C	51.038684	-42.370795	51.868410	C	51.370957	-42.610694	52.373622
C	49.360913	-42.066230	51.953971	C	49.534667	-42.317672	52.247313	C	49.866784	-42.655945	52.758421
O	48.826304	-42.695036	52.909174	O	49.139277	-43.172725	53.088140	O	49.565659	-43.357181	53.762646
O	48.787271	-41.329273	51.099816	O	48.839529	-41.447053	51.647393	O	49.083443	-42.009869	52.002365
C	50.753545	-42.800763	49.289231	C	50.601992	-42.321903	49.348652	C	50.996428	-43.097426	49.894959
C	51.973663	-42.129347	48.736596	C	51.773252	-41.749748	48.611185	C	52.095295	-42.376842	49.170364
N	54.346051	-40.733167	47.599356	N	54.013054	-40.676275	46.950279	N	54.228444	-40.761027	47.746933
C	53.039206	-40.570142	47.174751	C	52.683091	-40.322472	46.822371	C	52.893229	-40.777389	47.436088
C	52.958303	-39.529907	46.197083	C	52.506326	-39.400128	45.746386	C	52.637805	-39.875436	46.348001
C	54.224738	-38.992937	46.073714	C	53.751067	-39.153479	45.220112	C	53.840226	-39.277626	46.025762
C	55.083508	-39.736013	46.936297	C	54.689193	-39.916964	45.979336	C	54.834779	-39.837809	46.891238
N	56.859854	-41.514241	48.475395	N	56.644470	-41.402887	47.660783	N	56.957090	-41.384101	48.339026
C	57.295744	-40.399218	47.748414	C	56.973006	-40.444460	46.700711	C	57.200004	-40.300260	47.497474
C	58.721907	-40.300409	47.807698	C	58.376160	-40.211365	46.706286	C	58.610635	-40.090447	47.396071
C	59.162941	-41.359913	48.571185	C	58.918185	-41.037416	47.675343	C	59.222251	-41.059803	48.170811
C	58.000958	-42.097855	48.970176	C	57.839143	-41.784039	48.233009	C	58.177822	-41.859922	48.740632
C	52.840247	-39.229452	50.941678	C	52.840247	-39.229452	50.941678	C	52.840247	-39.229452	50.941678
C	53.878954	-40.134107	51.591330	C	54.097499	-40.001289	51.313386	C	53.928928	-39.816954	51.828877
S	55.339710	-40.448438	50.551069	S	55.329301	-40.008710	49.960554	S	55.518839	-40.106350	50.954090
H	56.048365	-45.855975	46.615992	H	56.097355	-45.528220	46.796138	H	56.680685	-45.615382	46.599799
H	49.402172	-52.501911	49.911214	H	49.303987	-52.431320	49.588355	H	49.271034	-52.263454	49.422816
H	51.165011	-52.650315	50.038984	H	50.924584	-52.713500	50.249683	H	50.742876	-52.936302	50.146362
H	50.406232	-52.376367	48.455395	H	50.717216	-52.373958	48.517074	H	50.798971	-52.217509	48.522891
H	49.628264	-50.098195	49.223178	H	49.907746	-50.050514	49.064833	H	50.242261	-49.954942	49.514176
H	50.370850	-50.377203	50.805995	H	50.093460	-50.384410	50.794720	H	50.199811	-50.676274	51.129692
H	52.619205	-50.576773	49.710338	H	52.541661	-50.722814	50.485863	H	52.610313	-51.321604	50.906844
H	51.864153	-50.245134	48.128462	H	52.367363	-50.429391	48.734157	H	52.639826	-50.598523	49.277182
H	54.492829	-47.743232	47.769866	H	55.238451	-48.193061	49.726362	H	55.600070	-48.800029	50.283266
H	53.993887	-49.356354	48.212282	H	54.409024	-49.715788	49.647540	H	54.671928	-50.244214	50.124367
H	53.651963	-46.049637	49.389378	H	54.050585	-46.297212	50.403992	H	54.665246	-46.900268	51.204681
H	52.010246	-46.152618	49.720160	H	52.377376	-46.312090	50.485466	H	52.967038	-46.803842	51.490307
H	52.139540	-46.493942	41.525961	H	52.093797	-46.648228	41.451827	H	52.106047	-46.874711	41.383069
H	51.602082	-46.574126	43.213149	H	51.602268	-46.486074	43.149767	H	51.745804	-46.243156	42.999531
H	54.098022	-46.159469	43.083994	H	54.105727	-46.032737	42.824166	H	54.269368	-46.311312	42.491569
H	54.292902	-47.615137	42.109577	H	54.286845	-47.651025	42.153330	H	54.141050	-48.055922	42.288443
H	53.397769	-49.000187	44.023247	H	53.442089	-48.612481	44.355712	H	53.242542	-48.175416	44.705202
H	53.297437	-47.552167	45.016898	H	53.423677	-46.987086	45.022687	H	53.683174	-46.476858	44.874171

H	54.421038	-46.162618	45.975448	H	54.489279	-46.071596	46.443442	H	54.957981	-45.824378	46.373043
H	57.723060	-48.433637	45.055707	H	57.871839	-47.699858	44.832500	H	57.792070	-48.283739	44.741441
H	57.786041	-47.159158	46.232298	H	57.887590	-46.460609	46.091200	H	58.143569	-47.126695	45.990638
H	57.307877	-45.233104	41.587102	H	57.275077	-45.240658	41.598743	H	57.325837	-45.233024	41.580521
H	56.989927	-45.539429	43.307079	H	57.011676	-45.533435	43.328777	H	56.972067	-45.532610	43.294048
H	58.657180	-45.416370	42.713469	H	58.661375	-45.415977	42.681440	H	58.652777	-45.422605	42.734319
H	58.314067	-42.967147	42.197079	H	58.203441	-42.954749	42.103178	H	58.261444	-42.959241	42.150551
H	56.610509	-43.096507	42.594992	H	56.574865	-43.118138	42.752603	H	56.590918	-43.106442	42.667191
H	57.206932	-43.653809	44.982731	H	57.562914	-43.716232	45.007177	H	57.420218	-43.717031	45.006578
H	57.762187	-42.033207	44.490252	H	57.897200	-42.061176	44.492366	H	57.794791	-42.049660	44.501240
H	60.067948	-42.815615	44.273768	H	60.197865	-42.627487	43.867981	H	60.119460	-42.656329	44.004317
H	59.568170	-44.509848	44.459192	H	59.883497	-44.365923	44.037206	H	59.775679	-44.381640	44.246340
H	59.341428	-42.446050	46.599573	H	59.785193	-42.425472	46.278543	H	59.604489	-42.328218	46.393444
H	60.411175	-43.709901	46.521020	H	61.016712	-43.510771	45.969899	H	60.806022	-43.457243	46.185923
H	51.274337	-43.488122	40.327547	H	52.054070	-43.311946	39.996934	H	51.261116	-43.492688	40.348730
H	52.572617	-42.279540	40.247165	H	52.181227	-41.718241	40.768938	H	52.568159	-42.297599	40.231270
H	51.135940	-41.975827	41.249002	H	50.748226	-42.728237	41.050407	H	51.148123	-41.963538	41.243769
H	53.193393	-44.220863	41.768113	H	53.612102	-43.476867	41.910488	H	53.181722	-44.224823	41.752186
H	51.778232	-43.875218	42.769098	H	52.177081	-44.451641	42.175469	H	51.764792	-43.892052	42.742001
H	52.706177	-41.530857	43.161821	H	51.264403	-42.615076	43.692490	H	52.730720	-41.637547	43.342570
H	54.164505	-42.004248	42.282379	H	52.823087	-41.780728	43.538917	H	54.197931	-42.044830	42.434818
H	54.587604	-43.809328	44.024623	H	53.993679	-43.869521	44.380825	H	54.570576	-44.039348	43.917561
H	53.136090	-43.269347	44.899731	H	52.414415	-44.678424	44.482719	H	53.005055	-43.743472	44.698953
H	55.602926	-41.701539	44.409880	H	53.426720	-42.455352	46.178297	H	55.479588	-42.174905	45.013547
H	54.946891	-42.140643	45.883253	H	52.863077	-43.998631	46.619778	H	54.469084	-42.919107	46.157886
H	58.986022	-43.812632	49.768265	H	59.011254	-43.180887	49.339601	H	59.376921	-43.418223	49.569783
H	53.185016	-44.509266	52.155418	H	53.300958	-44.200622	51.835477	H	53.874728	-44.490685	52.540384
H	50.968225	-41.065717	47.227329	H	50.630923	-40.499996	47.368644	H	50.882840	-41.408386	47.759837
H	56.900995	-38.740945	46.482377	H	56.452224	-39.122776	45.123250	H	56.531010	-38.816887	46.135670
H	56.864859	-46.908104	49.041706	H	57.448400	-46.431170	49.079180	H	57.517129	-46.582940	49.194771
H	55.405699	-45.919378	49.100160	H	55.748628	-45.937622	49.246486	H	55.902940	-46.049625	49.710303
H	55.673915	-47.205731	50.322713	H	56.559264	-46.900758	50.535583	H	56.883949	-47.151000	50.742771
H	58.707639	-45.230791	51.762831	H	58.766608	-44.069564	51.716032	H	59.409028	-44.581929	51.796221
H	58.044474	-46.851690	51.709640	H	58.360527	-45.743446	52.020548	H	58.932472	-46.253412	51.999520
H	50.555091	-45.323468	50.180125	H	50.859007	-45.066394	49.643628	H	51.507976	-45.691325	50.712806
H	49.589310	-44.522790	51.407826	H	49.618348	-44.524960	50.792612	H	50.201064	-45.078626	51.745140
H	51.172501	-45.145832	51.860638	H	51.153409	-45.091354	51.430228	H	51.778651	-45.359750	52.470668
H	51.327656	-41.283741	51.482272	H	51.427809	-41.349729	51.777379	H	51.629358	-41.590718	52.061231
H	51.345686	-42.572166	52.719822	H	51.599013	-42.896620	52.650933	H	51.987152	-42.888545	53.237511
H	52.042571	-39.208839	45.710864	H	51.551059	-38.983007	45.444417	H	51.662933	-39.693937	45.906476
H	54.544597	-38.168229	45.444428	H	54.017685	-38.487979	44.405020	H	54.030004	-38.530519	45.261300
H	59.309650	-39.520633	47.333479	H	58.887161	-39.496386	46.069292	H	59.084271	-39.300374	46.821485
H	60.181612	-41.608273	48.854736	H	59.949814	-41.097206	48.012086	H	60.283725	-41.189898	48.363181
H	52.404418	-39.705263	50.055185	H	52.337141	-39.679817	50.078695	H	52.572890	-39.912802	50.127908
H	53.456054	-41.093669	51.910535	H	53.870646	-41.039581	51.582616	H	53.622486	-40.774310	52.267187
H	54.308662	-39.661296	52.487442	H	54.600512	-39.541144	52.173665	H	54.176661	-39.138314	52.654391
H	51.203383	-48.207878	50.089755	H	51.216824	-48.233667	50.168174	H	51.700716	-48.762773	51.353374
H	55.751267	-48.906217	44.021653	H	55.839949	-48.470180	44.092233	H	55.618242	-48.643394	44.176152
H	58.749271	-44.038612	46.671574	H	59.461062	-44.072035	46.387751	H	59.222356	-43.973399	46.552140
H	54.194643	-41.005223	44.968294	H	51.822161	-42.810087	46.090448	H	53.998105	-41.510442	45.361255
H	52.028850	-39.011974	51.648679	H	52.135071	-39.212775	51.784471	H	51.937090	-39.041059	51.538759
H	53.289411	-38.278321	50.630314	H	53.083321	-38.191027	50.683668	H	53.163862	-38.279866	50.496984
O	52.742278	-45.420892	46.384896	O	52.835588	-45.679192	47.350064	O	53.910312	-44.214078	47.306679
H	52.568646	-45.693073	47.316884	H	52.982739	-45.944985	48.295926	H	54.013937	-43.832206	48.211955
H	51.876548	-45.468660	45.945082	H	52.010484	-46.129925	47.095428	H	52.941219	-44.268872	47.213140
O	57.494875	-44.988161	47.224013	O	58.295231	-45.023861	47.156056	O	58.150044	-44.957652	47.311927
H	57.043803	-44.309327	47.764702	H	57.766670	-44.269600	47.488755	H	57.707236	-44.268906	47.851102
H	58.081570	-45.508855	47.987431	H	58.814449	-45.310264	48.060995	H	58.781614	-45.402640	48.082519

H	51.805009	-48.065356	42.272830	H	51.832925	-48.093925	42.443086	H	51.681249	-47.991008	42.696310
H	56.366657	-44.519451	52.594963	H	56.340215	-43.786826	52.315694	H	57.055375	-44.146026	52.752970
H	55.338049	-45.925830	52.200104	H	55.566118	-45.364307	52.057011	H	56.194192	-45.685936	52.526177
H	50.467028	-43.647996	48.644968	H	50.017463	-42.978689	48.687568	H	50.643182	-43.950671	49.294834
H	49.894899	-42.121518	49.365811	H	49.913129	-41.549723	49.720262	H	50.130019	-42.458793	50.112156

Table S8. Cartesian coordinates (Å) of the heme species (Fe²⁺ & Fe³⁺) with ligands (and without the cubane cluster) optimized at DFT (BP86 functional) using TZ2P basis sets. S is the spin state of the species.

Heme (Fe ²⁺) with HSO ₃ ⁻											
S=0				S=1				S=2			
C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000
C	50.847628	5.820518	71.412240	C	50.881592	5.807970	71.413850	C	50.773203	5.820291	71.284222
C	51.401352	6.047370	70.004363	C	51.476031	6.004202	70.018816	C	51.492093	5.910744	69.936644
N	51.836944	7.438891	69.860476	N	51.958263	7.379944	69.868506	N	51.839424	7.305302	69.651701
C	52.601541	7.926852	68.875050	C	52.773948	7.818547	68.903395	C	52.793206	7.728734	68.814021
N	52.950023	7.165172	67.832933	N	53.143275	7.021200	67.897097	N	53.425289	6.883528	67.994469
N	53.077420	9.180679	68.942872	N	53.273885	9.063442	68.954943	N	53.151226	9.022072	68.815280
C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000
C	53.718495	2.555365	63.476468	C	53.716799	2.571825	63.457739	C	53.746776	2.177729	63.413382
C	54.180061	2.547778	64.943835	C	54.202150	2.537093	64.917056	C	54.242847	1.981321	64.860107
N	55.427842	3.279627	65.161458	N	55.445076	3.277355	65.131017	N	55.559479	2.562123	65.110567
C	55.497843	4.617541	65.074872	C	55.499719	4.617799	65.092355	C	55.764253	3.888365	65.155882
N	54.378283	5.340759	64.989804	N	54.369381	5.330304	65.039902	N	54.721737	4.721779	65.097743
N	56.682261	5.241770	65.068365	N	56.675051	5.255430	65.112974	N	57.000123	4.383603	65.275005
C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000
C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000
C	57.500151	6.228527	61.403919	C	57.460772	6.227937	61.400015	C	57.607143	6.220954	61.419759
C	58.790317	6.647973	62.098539	C	58.740334	6.674347	62.097505	C	58.994768	6.592715	61.928337
N	58.653058	8.014289	62.690010	N	58.578851	8.040344	62.682204	N	58.937057	7.840311	62.747499
C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000
C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000
C	53.181875	5.724870	60.171214	C	53.057986	5.783046	60.244515	C	53.149149	5.755903	60.338783
C	53.761180	6.155764	61.501897	C	53.694494	6.142443	61.572494	C	53.802423	5.944300	61.704713
N	54.337383	7.527291	61.463420	N	54.093055	7.570265	61.654344	N	54.326163	7.317789	61.950778
Fe	55.359214	10.915575	64.364410	Fe	55.332627	10.957020	64.395150	Fe	55.328463	10.943066	64.085480
C	57.889845	11.441675	66.574581	C	57.894702	11.432194	66.615426	C	57.883901	11.127743	66.409076
C	53.016632	11.389360	66.794250	C	53.043565	11.492788	66.838038	C	53.031457	11.315598	66.572272
C	52.825546	10.292187	62.089474	C	52.802053	10.284482	62.151141	C	52.852832	10.028359	61.882386
C	57.638629	10.814417	61.783659	C	57.612419	10.818300	61.799021	C	57.670103	10.560893	61.577180
N	55.468828	11.381414	66.286884	N	55.475052	11.437916	66.333562	N	55.468782	11.147930	66.136839
C	56.581411	11.603883	67.019460	C	56.602590	11.621315	67.068847	C	56.587098	11.278749	66.880633
C	56.270043	12.115557	68.421692	C	56.295417	12.098242	68.492992	C	56.279562	11.741996	68.308623
C	56.701773	11.147314	69.551935	C	56.706161	11.085925	69.590037	C	56.632580	10.703966	69.400490
C	56.851337	13.542518	68.668796	C	56.886428	13.509319	68.784206	C	56.928615	13.123501	68.621918
C	58.349776	13.728755	69.040888	C	58.394298	13.675137	69.131797	C	58.437231	13.224568	68.983018
O	59.151858	12.750457	68.966176	O	59.171882	12.676655	69.091775	O	59.180626	12.199313	68.918158
O	58.637739	14.905362	69.399660	O	58.710034	14.858530	69.443058	O	58.796271	14.385005	69.328849
C	54.786142	12.160259	68.345306	C	54.808839	12.167007	68.419899	C	54.796226	11.874894	68.218616
C	54.357732	11.672809	67.137545	C	54.387345	11.733426	67.183064	C	54.375523	11.488169	66.976328
N	53.339251	10.735949	64.470167	N	53.359217	10.794163	64.523995	N	53.396569	10.633696	64.241782
C	52.575058	10.938435	65.577896	C	52.597168	11.003933	65.643956	C	52.613780	10.861097	65.362103
C	51.087283	10.660256	65.317441	C	51.121907	10.682502	65.420385	C	51.130682	10.583569	65.104761
C	50.536889	9.596752	66.286862	C	50.646440	9.571823	66.383279	C	50.551750	9.578163	66.122192
C	50.286757	11.981467	65.465503	C	50.255955	11.956685	65.612111	C	50.335218	11.917949	65.176343
C	48.756044	11.899995	65.246040	C	48.732395	11.796789	65.372670	C	48.809447	11.828320	64.924095
O	48.092956	12.835990	65.784280	O	48.020486	12.704453	65.893312	O	48.132925	12.773513	65.426589
O	48.290453	10.952515	64.548554	O	48.324642	10.819304	64.680489	O	48.364899	10.865222	64.234550
C	51.141248	10.233753	63.881155	C	51.162026	10.272067	63.989309	C	51.199245	10.082360	63.699787
C	52.442363	10.374382	63.445582	C	52.454378	10.410693	63.506039	C	52.492071	10.218303	63.231811
N	55.259792	10.573359	62.379974	N	55.233124	10.565199	62.397993	N	55.278718	10.342730	62.150185
C	54.098978	10.447428	61.610986	C	54.082920	10.428126	61.643213	C	54.137004	10.151236	61.382361
C	54.437151	10.421969	60.199482	C	54.410586	10.352583	60.238409	C	54.493914	9.968747	59.998581
C	55.791523	10.526392	60.117882	C	55.774463	10.455752	60.144695	C	55.861013	10.064779	59.924573
C	56.293543	10.637288	61.475074	C	56.275938	10.610825	61.485077	C	56.339297	10.318405	61.254787

H	58.344724	10.870302	60.955168	H	58.321734	10.863373	60.971437	H	58.393522	10.568586	60.761779
H	57.783117	10.975333	69.522985	H	57.790149	10.928744	69.570101	H	57.721794	10.608046	69.480679
H	56.131402	10.209157	69.485154	H	56.156780	10.142664	69.462995	H	56.154687	9.739870	69.185165
H	56.461765	11.600449	70.522927	H	56.442498	11.492524	70.575726	H	56.254455	11.062178	70.367454
H	56.654570	14.161808	67.781571	H	56.675222	14.163296	67.926319	H	56.751869	13.796985	67.771004
H	56.270943	13.993609	69.486202	H	56.328735	13.933694	69.632145	H	56.379398	13.560380	69.468689
H	54.141141	12.480424	69.159413	H	54.161518	12.463465	69.240931	H	54.155645	12.172135	69.044381
H	51.136245	8.679193	66.239399	H	51.291967	8.687326	66.310750	H	51.155979	8.662832	66.159292
H	49.499702	9.364266	66.020540	H	49.618383	9.291443	66.129225	H	49.525876	9.323037	65.833925
H	50.557887	9.977456	67.318108	H	50.666331	9.936116	67.419496	H	50.532097	10.024190	67.126141
H	50.681296	12.718013	64.748961	H	50.614708	12.740238	64.927583	H	50.748580	12.618701	64.435328
H	50.469053	12.398240	66.466755	H	50.402037	12.344010	66.630017	H	50.497284	12.375620	66.162332
H	50.263136	10.122604	63.253979	H	50.274527	10.067736	63.398982	H	50.323319	9.868744	63.096208
H	53.710916	10.346614	59.395111	H	53.681932	10.247710	59.439275	H	53.782604	9.800378	59.195254
H	56.414943	10.562742	59.228925	H	56.391946	10.465313	59.250827	H	56.493935	10.004574	59.043772
H	60.347317	11.095632	62.687335	H	60.312413	11.103179	62.684534	H	60.343188	10.953693	62.500678
H	60.485068	11.318198	65.399183	H	60.464453	11.316881	65.400974	H	60.450877	11.120259	65.219650
H	55.949135	8.487968	66.913425	H	56.082467	8.532353	66.983838	H	56.818367	7.929177	67.315417
H	52.688682	12.728112	62.329088	H	52.695672	12.718404	62.358446	H	52.751670	12.714121	62.343122
H	53.085328	13.330912	64.759476	H	53.108074	13.419218	64.773521	H	53.162183	13.365806	64.748852
H	53.743004	14.888361	64.258020	H	53.779716	14.942830	64.198883	H	53.740191	14.953324	64.217719
H	51.459929	8.110298	70.522271	H	51.601201	8.070010	70.521965	H	51.270340	8.019671	70.096449
H	56.297557	2.760089	65.195020	H	56.320296	2.766503	65.149116	H	56.367269	1.951924	65.152296
H	57.912343	8.060888	63.459383	H	57.842244	8.078815	63.449559	H	58.352768	7.672544	63.622582
H	53.648770	8.226946	61.147080	H	53.288093	8.210121	61.525126	H	53.577917	8.043894	61.891313
H	51.847268	14.234639	62.757559	H	51.844659	14.228592	62.759610	H	51.821639	14.165590	62.783588
H	53.373264	14.288210	61.836807	H	53.356957	14.270786	61.815352	H	53.310158	14.315448	61.816092
O	51.837723	7.256250	64.050396	O	51.754001	7.168230	64.098476	O	52.247171	7.198470	64.286132
H	52.737646	7.633154	64.179269	H	52.589245	7.653630	64.285607	H	53.113201	7.502638	64.632773
H	51.315887	8.086733	63.928720	H	51.117517	7.900801	63.976331	H	51.795395	8.039786	64.038850
O	57.368933	8.615719	67.653783	O	57.514165	8.648249	67.608102	O	58.245564	8.466240	67.783955
H	57.750798	9.402512	67.193979	H	57.788885	9.536128	67.243483	H	58.275761	9.340610	67.311669
H	57.251444	8.938496	68.567864	H	57.470208	8.810307	68.568772	H	58.238805	8.720076	68.725446
H	51.961832	1.310000	63.815036	H	51.980546	1.301169	63.806901	H	51.754224	1.386935	63.803422

Heme (Fe³⁺) with HSO₃⁻

S=1/2			S=3/2			S=5/2					
C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000
C	50.927584	5.785741	71.393806	C	50.915352	5.794959	71.418345	C	50.494724	5.669415	70.802581
C	51.551992	5.932944	70.006033	C	51.552697	5.966986	70.039175	C	51.817988	5.682479	70.044831
N	52.077314	7.292402	69.834137	N	52.060924	7.335408	69.889870	N	51.895765	6.864880	69.186611
C	52.893114	7.693965	68.857144	C	52.880685	7.761881	68.926829	C	52.916363	7.148814	68.372783
N	53.241856	6.867781	67.865667	N	53.252762	6.954602	67.928387	N	53.984191	6.337328	68.314444
N	53.416113	8.932988	68.873533	N	53.381913	9.009354	68.964103	N	52.897815	8.244204	67.608585
C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000
C	53.717382	2.540364	63.506130	C	53.714059	2.572748	63.478184	C	53.744608	2.172746	63.403566
C	54.136800	2.574074	64.984582	C	54.175867	2.543108	64.943762	C	54.251208	2.037914	64.853167
N	55.391499	3.292424	65.209260	N	55.434614	3.256516	65.162844	N	55.537228	2.691000	65.078896
C	55.486124	4.624156	65.095927	C	55.522108	4.592028	65.113245	C	55.678345	4.023965	65.091307
N	54.380521	5.365180	64.966537	N	54.410283	5.334448	65.056905	N	54.594630	4.813443	65.025024
N	56.681313	5.228823	65.109930	N	56.715434	5.199958	65.125036	N	56.892216	4.577077	65.156627
C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000
C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000
C	57.540626	6.228594	61.405635	C	57.524895	6.230827	61.403745	C	57.602451	6.217675	61.414649
C	58.845918	6.618328	62.088468	C	58.835746	6.632188	62.068962	C	58.946329	6.563036	62.042878
N	58.745031	7.999408	62.661577	N	58.731554	8.001735	62.669008	N	58.818828	7.824779	62.838212
C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000
C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000
C	53.226979	5.704409	60.170974	C	53.139823	5.749157	60.218621	C	53.096832	5.779695	60.394097

H	53.157242	6.089763	62.288835	H	53.144517	6.069180	62.307647	H	53.307476	5.771620	62.436328
H	55.095659	7.684694	60.720607	H	55.011587	7.746739	60.729259	H	55.179083	7.557071	60.993284
H	54.720303	7.769141	62.427259	H	54.690677	7.773164	62.444681	H	55.048326	7.381646	62.695023
H	58.728752	11.491160	67.245379	H	58.789798	11.414357	67.161955	H	59.368740	11.314051	65.516491
H	52.332057	11.400562	67.375896	H	52.398574	11.540516	67.385432	H	53.237657	10.944258	67.364608
H	52.231875	10.172174	61.113496	H	52.154409	10.139413	61.170283	H	51.513104	9.825783	61.309284
H	58.547541	10.922206	60.850000	H	58.491404	10.904574	60.766383	H	57.653645	9.768852	59.529918
H	57.813023	10.333653	69.247062	H	57.842533	10.327521	69.205349	H	59.228606	10.406716	67.751553
H	56.208000	9.559751	68.929121	H	56.190852	9.630028	68.948626	H	57.782025	9.334199	67.781045
H	56.422615	10.660994	70.307869	H	56.502712	10.743319	70.299186	H	58.089585	10.481130	69.118681
H	56.676804	13.795796	68.191640	H	56.777817	13.830117	68.127208	H	57.229137	13.558215	67.030415
H	56.242395	13.272677	69.808018	H	56.440370	13.325309	69.772586	H	57.594070	13.049916	68.670684
H	54.162739	11.864733	69.125196	H	54.245775	11.988969	69.116533	H	55.484299	11.409497	68.629109
H	51.129035	8.630697	65.945080	H	51.170331	8.716411	66.017338	H	51.518269	8.419666	66.202866
H	49.528768	9.384993	65.717795	H	49.571140	9.472789	65.788860	H	49.987870	9.321256	66.368749
H	50.579716	9.944815	67.039567	H	50.622391	10.036502	67.106206	H	51.359259	9.733161	67.422374
H	50.837690	12.691855	64.492043	H	50.878055	12.789889	64.577012	H	51.289954	12.555972	64.950615
H	50.583181	12.369884	66.202021	H	50.601749	12.445420	66.280289	H	51.297686	12.163031	66.663228
H	50.417312	10.145953	62.950253	H	50.411426	10.128963	63.067546	H	50.273237	9.889862	63.546839
H	53.963937	10.276817	59.205579	H	53.872624	10.223979	59.193129	H	52.752856	9.604348	59.003047
H	56.671459	10.519646	59.094288	H	56.585653	10.473223	59.030446	H	55.371669	9.481092	58.268430
H	60.505883	11.196024	62.625738	H	60.458090	11.177125	62.503103	H	59.941046	10.244654	60.730763
H	60.583023	11.380212	65.347848	H	60.580629	11.310019	65.229085	H	60.654052	10.920001	63.282547
H	52.690889	12.731663	62.314740	H	52.694350	12.723528	62.339031	H	52.604426	12.750092	62.296651
H	53.213672	13.286296	64.729698	H	53.278652	13.371062	64.735730	H	53.664012	13.143013	64.551606
H	53.821378	14.866549	64.227369	H	53.890794	14.916363	64.147298	H	54.198733	14.746639	64.018658
H	51.233992	7.393341	69.056597	H	51.246547	7.447445	69.135574	H	51.658012	7.023558	68.806613
H	56.307976	2.767880	65.081384	H	56.320901	2.745660	65.085251	H	56.049959	1.970424	65.604476
H	58.007866	8.108031	63.369410	H	57.965804	8.105991	63.379163	H	58.762813	7.290745	63.696862
H	53.620381	8.202517	61.251382	H	53.547949	8.221238	61.335409	H	53.782674	7.987068	61.751399
H	51.847552	14.214547	62.823875	H	51.848382	14.205733	62.848638	H	51.922043	14.201518	63.071054
H	53.317477	14.316814	61.820094	H	53.281161	14.304879	61.792523	H	53.127460	14.364148	61.766650
O	52.051343	7.332982	63.912929	O	52.021625	7.304887	64.001655	O	52.735618	7.215946	64.324317
H	52.979434	7.636922	64.059720	H	52.947732	7.637283	64.110543	H	53.665768	7.517285	64.462127
H	51.601413	8.209294	63.749799	H	51.535992	8.143569	63.828079	H	52.238652	8.039851	64.118643
O	56.890454	7.190187	67.951552	O	56.884307	7.263588	67.988983	O	57.353450	6.505070	68.488465
H	56.471961	7.703855	67.193436	H	56.455696	7.754787	67.222843	H	57.091696	6.991251	67.640917
H	57.331422	7.871980	68.487877	H	57.327990	7.963843	68.499985	H	57.699225	7.201891	69.072228
H	52.060914	1.247896	63.721225	H	52.042240	1.258661	63.740449	H	51.717588	1.407575	63.804762

Heme (Fe³⁺) with SO₃²⁻

S=1/2			S=3/2			S=5/2					
C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000
C	50.520900	5.631474	70.749612	C	50.522500	5.621000	70.735579	C	50.630703	5.562625	70.686235
C	51.965098	5.771650	70.278593	C	51.968666	5.758661	70.270612	C	52.040979	5.468093	70.112556
N	52.110303	6.933079	69.403459	N	52.116995	6.913236	69.387478	N	52.320626	6.584693	69.211067
C	53.244160	7.263357	68.763255	C	53.258513	7.252929	68.766619	C	53.514628	6.796700	68.627245
N	54.335838	6.503660	68.911936	N	54.348578	6.491589	68.917962	N	54.519081	5.940591	68.855029
N	53.285227	8.350529	67.986247	N	53.306964	8.350317	68.004181	N	53.696350	7.845699	67.824499
C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000
C	53.707645	2.591832	63.513446	C	53.699222	2.639272	63.486034	C	53.732219	2.476834	63.478175
C	54.133704	2.604722	64.990328	C	54.172180	2.602539	64.947916	C	54.214666	2.299127	64.926274
N	55.395499	3.309222	65.222039	N	55.438708	3.304845	65.161229	N	55.546063	2.854744	65.165669
C	55.509213	4.641901	65.062488	C	55.542740	4.643476	65.060923	C	55.789411	4.180366	65.156202
N	54.417402	5.397213	64.974276	N	54.447342	5.400055	65.053141	N	54.777948	5.045328	65.207353
N	56.715470	5.216866	64.982054	N	56.744769	5.225438	64.966328	N	57.044688	4.640473	65.113892
C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000
C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000
C	57.553369	6.238973	61.382825	C	57.524313	6.242323	61.376708	C	57.658041	6.229684	61.394270

C	58.872849	6.663863	62.016843	C	58.846241	6.704228	61.979380	C	59.061168	6.588898	61.868733
N	58.760561	8.056896	62.548043	N	58.718905	8.098180	62.505501	N	59.036838	7.894700	62.591304
C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000
C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000
C	53.235892	5.692143	60.128298	C	53.176797	5.724902	60.157567	C	53.215345	5.719749	60.246713
C	53.861775	6.137852	61.430969	C	53.843337	6.136428	61.452647	C	53.927041	5.977107	61.567726
N	54.461472	7.496523	61.348221	N	54.365033	7.526461	61.412486	N	54.464857	7.359205	61.700926
Fe	55.448460	10.977397	64.177943	Fe	55.412123	11.037968	64.131235	Fe	55.542636	11.192275	63.946264
C	58.001370	11.307560	66.403586	C	57.980647	11.352304	66.370511	C	58.350007	11.350110	65.971472
C	53.137759	11.392070	66.636040	C	53.131775	11.389802	66.644760	C	53.530004	10.986421	66.717327
C	52.946444	10.297828	61.917714	C	52.882746	10.275878	61.924493	C	52.907502	10.202743	61.931874
C	57.730079	10.925801	61.588755	C	57.682727	10.932919	61.539111	C	57.688637	10.667384	61.208409
N	55.582287	11.339247	66.113756	N	55.558630	11.353670	66.133389	N	55.921981	11.199572	66.031484
C	56.701258	11.424263	66.868380	C	56.696621	11.446159	66.863807	C	57.108349	11.296555	66.632460
C	56.397999	11.707772	68.333390	C	56.400163	11.718166	68.338831	C	56.960366	11.336155	68.145844
C	56.795134	10.524411	69.251893	C	56.817649	10.530161	69.239337	C	57.658713	10.135027	68.828862
C	56.994967	13.056415	68.840865	C	56.990115	13.067607	68.840479	C	57.413566	12.698013	68.770035
C	58.502502	13.158644	69.212369	C	58.511872	13.208647	69.134629	C	58.926717	13.008102	68.953567
O	59.281394	12.185000	68.998405	O	59.280910	12.212257	69.012442	O	59.802062	12.250268	68.445877
O	58.811484	14.271312	69.723509	O	58.840704	14.372246	69.502971	O	59.134056	14.054255	69.629753
C	54.921005	11.807005	68.272499	C	54.915071	11.805832	68.292986	C	55.479249	11.229757	68.267092
C	54.489184	11.545960	66.999822	C	54.478801	11.549741	67.009967	C	54.913226	11.145712	67.020430
N	53.483837	10.777689	64.304956	N	53.434764	10.789608	64.296988	N	53.605974	10.678273	64.281905
C	52.697086	10.981260	65.417395	C	52.677080	10.981093	65.422898	C	52.957545	10.748798	65.499979
C	51.214188	10.743960	65.138403	C	51.191244	10.732533	65.175905	C	51.444339	10.539347	65.331716
C	50.602228	9.685673	66.078465	C	50.607104	9.675973	66.136506	C	50.873959	9.461657	66.272267
C	50.436089	12.085556	65.277608	C	50.412628	12.071309	65.334167	C	50.715166	11.891716	65.586556
C	48.920830	12.036412	64.959619	C	48.888358	12.020004	65.053237	C	49.178425	11.899891	65.385062
O	48.251199	12.986996	65.456599	O	48.235391	12.984170	65.546914	O	48.584416	12.867743	65.942652
O	48.484705	11.098527	64.231251	O	48.431154	11.069661	64.355834	O	48.653259	10.989156	64.682106
C	51.283099	10.327294	63.712697	C	51.232513	10.304031	63.751454	C	51.382741	10.190016	63.877959
C	52.587686	10.420517	63.276494	C	52.531589	10.416361	63.276106	C	52.637892	10.337212	63.323686
N	55.365546	10.620317	62.194994	N	55.314858	10.595574	62.161171	N	55.353711	10.462011	61.959158
C	54.212733	10.453970	61.428179	C	54.159259	10.434079	61.414843	C	54.136535	10.286602	61.312794
C	54.545094	10.417416	60.014989	C	54.481058	10.377623	60.010431	C	54.369048	10.121725	59.886799
C	55.893098	10.569961	59.929899	C	55.841266	10.519246	59.906467	C	55.716722	10.202555	59.692894
C	56.392960	10.710618	61.285417	C	56.351793	10.678051	61.238669	C	56.322423	10.441820	60.994786
N	57.447838	11.090026	64.022932	N	57.411885	11.152356	63.976898	N	57.615852	11.074064	63.629050
C	58.216054	11.082674	62.879469	C	58.176847	11.139925	62.819030	C	58.279562	10.980950	62.436124
C	59.621072	11.178287	63.214125	C	59.573363	11.256242	63.148310	C	59.711603	11.153903	62.652781
C	59.697668	11.221537	64.576199	C	59.654099	11.312419	64.515001	C	59.891467	11.317122	63.993409
C	58.341781	11.186492	65.072578	C	58.305104	11.261468	65.020352	C	58.575012	11.263637	64.611400
S	55.648298	8.730985	64.708313	S	55.679939	8.743785	64.746441	S	56.337386	8.294013	64.945135
O	56.993752	8.024851	64.465010	O	57.031009	8.059067	64.500370	O	57.590252	7.396667	64.684009
O	54.628227	7.886797	63.885620	O	54.661269	7.881089	63.950487	O	55.182145	7.509407	64.206134
O	55.318489	8.430437	66.155738	O	55.367572	8.485264	66.202259	O	56.038290	8.086935	66.429051
C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000
C	53.725163	13.901123	63.876635	C	53.675242	13.881922	63.913450	C	53.691993	13.960339	63.888331
S	55.419714	13.227594	63.696719	S	55.357839	13.177393	63.781636	S	55.438546	13.454450	63.634773
H	54.494510	6.391953	64.681239	H	54.514882	6.396393	64.765214	H	54.937645	6.043583	64.933180
H	49.288980	4.309850	71.959601	H	49.287190	4.310780	71.953905	H	49.314599	4.472945	72.032903
H	50.965219	4.443834	72.524751	H	50.959237	4.457071	72.527940	H	51.029970	4.380407	72.476254
H	50.587556	3.476826	71.082967	H	50.593631	3.470948	71.096143	H	50.412707	3.432335	71.105787
H	49.863566	5.570281	69.869271	H	49.869627	5.548689	69.853007	H	49.905805	5.572942	69.858539
H	50.234044	6.537302	71.303775	H	50.231621	6.532566	71.278013	H	50.524147	6.517880	71.220574
H	52.634009	5.877866	71.147511	H	52.633152	5.871210	71.142130	H	52.770875	5.481746	70.937501
H	52.261581	4.861237	69.732491	H	52.268414	4.845164	69.732097	H	52.157778	4.512566	69.574265
H	55.267998	6.818055	68.577752	H	55.283789	6.807910	68.594077	H	55.501086	6.168802	68.600880

H	54.313928	5.736787	69.571317	H	54.320442	5.718277	69.569425	H	54.377199	5.185417	69.513259
H	54.038730	8.472394	67.285047	H	54.069839	8.484761	67.316898	H	54.568158	7.969628	67.270752
H	52.439122	8.886792	67.830817	H	52.459872	8.882495	67.839884	H	52.941486	8.500256	67.652072
H	51.951567	2.207380	62.286628	H	51.924516	2.240328	62.292753	H	51.907420	2.329701	62.299478
H	51.598370	3.040587	63.812575	H	51.584689	2.997083	63.860732	H	51.670712	3.028638	63.912913
H	53.914819	3.578477	63.075691	H	53.858226	3.650749	63.087061	H	53.991215	3.490143	63.140819
H	54.331436	1.870892	62.967018	H	54.331071	1.965954	62.890404	H	54.282694	1.781163	62.829554
H	54.260324	1.585652	65.370459	H	54.316362	1.571163	65.286630	H	54.256128	1.238520	65.196018
H	53.351698	3.062397	65.615378	H	53.409856	3.033709	65.614528	H	53.503132	2.758548	65.629574
H	53.496797	4.982802	65.024037	H	53.529970	4.976564	65.089068	H	53.825911	4.707918	65.248125
H	57.547148	4.659886	65.127170	H	57.582189	4.664249	65.043450	H	57.812265	3.992380	64.998037
H	56.814445	6.246602	64.924450	H	56.842565	6.254810	64.934180	H	57.242760	5.659240	65.046476
H	57.618455	2.710566	61.198859	H	57.648403	2.711090	61.198463	H	57.579725	2.709089	61.202810
H	56.748601	3.692911	62.396402	H	56.732613	3.675931	62.375385	H	56.769225	3.716529	62.420558
H	58.524388	3.697541	62.360446	H	58.509229	3.713726	62.380978	H	58.542321	3.676612	62.334498
H	58.444101	4.788119	60.046573	H	58.454411	4.798512	60.058767	H	58.401461	4.747772	60.000073
H	56.688583	4.746716	60.099740	H	56.699705	4.732496	60.086718	H	56.652662	4.787033	60.148264
H	56.772408	6.272005	62.158392	H	56.756429	6.258539	62.165973	H	56.978876	6.265886	62.260409
H	57.300406	6.986138	60.612417	H	57.232473	6.977039	60.608743	H	57.333291	7.002459	60.678653
H	59.688888	6.638970	61.286505	H	59.645128	6.693241	61.229900	H	59.756434	6.663449	61.025342
H	59.144249	6.022246	62.861772	H	59.153613	6.073905	62.820656	H	59.450171	5.846087	62.573702
H	58.498986	8.740765	61.819562	H	58.411097	8.772392	61.784882	H	58.626589	8.647539	62.013721
H	59.640617	8.391272	62.955147	H	59.605438	8.458658	62.875031	H	59.974615	8.204657	62.862246
H	51.338536	2.899131	59.214882	H	51.378853	2.877166	59.202124	H	51.374433	2.882232	59.218410
H	52.563044	3.730578	58.233951	H	52.555100	3.775654	58.221072	H	52.553634	3.760327	58.221487
H	51.079542	4.581969	58.712707	H	51.047109	4.558202	58.738416	H	51.050154	4.557728	58.729097
H	53.263615	3.604018	60.659869	H	53.299108	3.626234	60.628654	H	53.282562	3.606797	60.626702
H	51.792220	4.454993	61.134920	H	51.802694	4.402664	61.148916	H	51.796182	4.390116	61.144253
H	52.508898	6.449643	59.796336	H	52.409424	6.467794	59.890440	H	52.468243	6.508095	60.067491
H	54.000091	5.610150	59.339664	H	53.909842	5.706768	59.336141	H	53.931849	5.752277	59.411643
H	54.655845	5.453330	61.755516	H	54.684036	5.476475	61.701655	H	54.769313	5.287192	61.704570
H	53.110355	6.194315	62.228750	H	53.128043	6.115963	62.284532	H	53.239363	5.856282	62.413240
H	55.268059	7.542777	60.719590	H	55.106048	7.668474	60.719606	H	55.145391	7.592476	60.969770
H	54.719799	7.801111	62.356103	H	54.691731	7.797220	62.403332	H	54.904624	7.501124	62.685924
H	58.789520	11.410891	67.151285	H	58.786737	11.454196	67.096816	H	59.208960	11.493646	66.630654
H	52.402980	11.573060	67.418702	H	52.397157	11.560607	67.429905	H	52.861980	11.030943	67.577021
H	52.134014	10.144640	61.208368	H	52.067340	10.124264	61.218262	H	52.039430	10.038962	61.293605
H	58.436250	10.995045	60.762047	H	58.384546	10.992227	60.707096	H	58.337562	10.643360	60.333700
H	57.876467	10.363163	69.202454	H	57.899315	10.376171	69.173401	H	58.741703	10.212025	68.696628
H	56.242816	9.624395	68.953994	H	56.266593	9.630584	68.938134	H	57.282782	9.203951	68.391066
H	56.526572	10.762982	70.289128	H	56.561342	10.755381	70.283108	H	57.430446	10.147173	69.902284
H	56.789326	13.837146	68.094983	H	56.723031	13.857420	68.124671	H	56.983258	13.520036	68.180318
H	56.436710	13.344139	69.743238	H	56.474723	13.324224	69.778556	H	56.956822	12.766636	69.766830
H	54.278126	12.001025	69.126605	H	54.275449	11.975417	69.154355	H	54.944401	11.217375	69.212614
H	51.157715	8.740720	66.020861	H	51.165888	8.733556	66.069964	H	51.388093	8.502159	66.130761
H	49.561579	9.503709	65.788578	H	49.562138	9.487013	65.867759	H	49.807649	9.324764	66.061773
H	50.608415	10.055560	67.114304	H	50.630171	10.049170	67.171044	H	50.975839	9.784821	67.318646
H	50.886222	12.831958	64.606973	H	50.841086	12.819168	64.650847	H	51.133240	12.656902	64.916191
H	50.568507	12.465779	66.299877	H	50.564663	12.455367	66.352197	H	50.940440	12.220479	66.611123
H	50.409215	10.142324	63.096655	H	50.346769	10.109228	63.156049	H	50.455802	10.006346	63.345390
H	53.818889	10.306974	59.214953	H	53.750085	10.257775	59.215826	H	53.590555	9.969282	59.144807
H	56.515189	10.615666	59.040658	H	56.450487	10.548624	59.007646	H	56.263598	10.139092	58.756635
H	60.426724	11.217674	62.486331	H	60.378193	11.290100	62.419138	H	60.464273	11.138516	61.869323
H	60.576930	11.305671	65.207270	H	60.536225	11.408601	65.140486	H	60.818614	11.471990	64.536633
H	52.686057	12.718211	62.369291	H	52.676698	12.721634	62.360335	H	52.839795	12.718007	62.322698
H	53.254898	13.440350	64.754200	H	53.174974	13.414170	64.769077	H	53.295483	13.381073	64.731005
H	53.870871	14.963481	64.121107	H	53.844134	14.936772	64.170577	H	53.710560	15.016022	64.188349
H	51.279501	7.478484	69.200110	H	51.294447	7.477854	69.203848	H	51.543933	7.171614	68.925785

H	56.250395	2.766051	65.258070	H	56.296312	2.764804	65.142723	H	56.342700	2.229185	65.134302
H	57.999394	8.125505	63.319955	H	57.991268	8.155448	63.305583	H	58.423007	7.785418	63.499953
H	53.780377	8.194211	61.019097	H	53.619485	8.209208	61.201465	H	53.712634	8.063663	61.633413
H	51.850294	14.219536	62.822710	H	51.855849	14.236342	62.798061	H	51.795770	14.060161	62.841268
H	53.294126	14.273190	61.780530	H	53.329615	14.273401	61.801185	H	53.213967	14.375429	61.808656
O	51.990168	7.246946	63.998840	O	52.009697	7.278804	64.029438	O	52.482281	7.237884	64.200389
H	52.881544	7.670575	64.063466	H	52.910061	7.678252	64.108854	H	53.407854	7.540091	64.374681
H	51.406171	8.007246	63.809681	H	51.449483	8.062972	63.855009	H	52.000816	8.069432	64.005427
O	56.874406	7.248563	67.912574	O	56.897664	7.242298	67.948939	O	57.187695	6.464518	68.141389
H	56.448223	7.754730	67.160114	H	56.487718	7.769478	67.203725	H	56.904957	7.094637	67.410604
H	57.357504	7.922067	68.422701	H	57.382326	7.900073	68.477986	H	57.660201	7.021266	68.783946
H	51.971828	1.305205	63.811021	H	52.020285	1.278286	63.776723	H	51.924786	1.281700	63.726654

Heme (Fe²⁺) with NO₂⁻

S=0			S=1			S=2					
C	50.331000	-52.045950	49.409000	C	50.331000	-52.045950	49.409000	C	50.331000	-52.045950	49.409000
C	50.396822	-50.546323	49.708313	C	50.426392	-50.562574	49.768531	C	50.482448	-50.589933	49.849349
C	51.806887	-49.981802	49.543993	C	51.841260	-50.013926	49.596134	C	51.896327	-50.060605	49.621234
N	51.801071	-48.536930	49.780645	N	51.862326	-48.582401	49.900560	N	51.965281	-48.647650	49.994420
C	52.843383	-47.718037	49.580179	C	52.892017	-47.758004	49.667220	C	52.991672	-47.826986	49.730296
N	54.014659	-48.214545	49.150403	N	54.028104	-48.231592	49.133588	N	54.082351	-48.290476	49.099551
N	52.710652	-46.407063	49.781148	N	52.788188	-46.460040	49.963274	N	52.937315	-46.543926	50.093394
C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410
C	53.686155	-46.947262	42.879566	C	53.697825	-46.920697	42.827988	C	53.704341	-46.913329	42.800063
C	54.073488	-48.069018	43.848485	C	54.141688	-48.040348	43.776280	C	54.171833	-48.029587	43.742101
N	55.347014	-47.850297	44.530194	N	55.405831	-47.774577	44.458860	N	55.428612	-47.741697	44.427193
C	55.499858	-47.016785	45.570613	C	55.520578	-46.960135	45.518910	C	55.522789	-46.951706	45.509970
N	54.458329	-46.337658	46.047829	N	54.446481	-46.337664	46.004830	N	54.435126	-46.381012	46.023296
N	56.719281	-46.830212	46.112644	N	56.727147	-46.733251	46.071971	N	56.727851	-46.702699	46.059264
C	57.624000	-44.932480	42.491060	C	57.624000	-44.932480	42.491060	C	57.624000	-44.932480	42.491060
C	57.584000	-43.404240	42.750400	C	57.584000	-43.404240	42.750400	C	57.584000	-43.404240	42.750400
C	57.414317	-43.052232	44.233883	C	57.351971	-43.047733	44.225719	C	57.245249	-43.032875	44.201541
C	58.582499	-43.463817	45.121559	C	58.494640	-43.418847	45.163540	C	58.309473	-43.409600	45.227464
N	58.348254	-42.965781	46.512029	N	58.207157	-42.886623	46.530640	N	57.939270	-42.853927	46.564270
C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430
C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930
C	52.751000	-42.494798	43.313259	C	52.682939	-42.511898	43.335672	C	52.453819	-42.630319	43.418778
C	53.926473	-43.028125	44.111809	C	53.852001	-43.021509	44.156153	C	53.568679	-43.122500	44.320351
N	53.988083	-42.465097	45.478608	N	53.878646	-42.457589	45.523285	N	53.467669	-42.635901	45.707715
Fe	55.035838	-42.249055	49.423530	Fe	54.964300	-42.294884	49.500603	Fe	54.864652	-42.280177	49.727043
C	57.428697	-44.067640	50.975502	C	57.424582	-44.214944	50.846678	C	57.463248	-44.203035	50.847963
C	52.571437	-43.688021	51.312651	C	52.642810	-43.725506	51.539705	C	52.710478	-43.871466	51.787232
C	52.655283	-40.584206	47.587608	C	52.505499	-40.750078	47.705951	C	52.278447	-40.943208	47.932421
C	57.473239	-40.253696	47.998347	C	57.311569	-40.201553	48.104173	C	57.056871	-40.116630	48.244713
N	55.031299	-43.603907	50.888256	N	55.047199	-43.696748	50.947160	N	55.079386	-43.779342	51.076112
C	56.108548	-44.241025	51.388728	C	56.147155	-44.378823	51.353503	C	56.216830	-44.433819	51.405279
C	55.756145	-45.135448	52.571635	C	55.838946	-45.297218	52.540370	C	55.994884	-45.391153	52.581876
C	56.057799	-46.630349	52.313706	C	56.028452	-46.798721	52.224826	C	56.189609	-46.878064	52.206777
C	56.428952	-44.646844	53.894901	C	56.622907	-44.883108	53.823335	C	56.851568	-44.997589	53.821889
C	57.926104	-44.946685	54.190182	C	58.129670	-45.242333	53.976964	C	58.377499	-45.302600	53.863604
O	58.660522	-45.482330	53.307274	O	58.743463	-45.841632	53.046441	O	58.937675	-45.899617	52.898149
O	58.284222	-44.607018	55.353083	O	58.614270	-44.884834	55.087273	O	58.934051	-44.911650	54.928046
C	54.289219	-44.895528	52.639556	C	54.394951	-44.990087	52.733251	C	54.555981	-45.117189	52.867931
C	53.901895	-44.036280	51.644800	C	53.980130	-44.088035	51.772484	C	54.067060	-44.210090	51.953102
N	53.024747	-42.222112	49.413474	N	52.977568	-42.323838	49.574417	N	52.900892	-42.454287	49.804867
C	52.193928	-42.916533	50.255326	C	52.197218	-42.997941	50.465873	C	52.190422	-43.161663	50.736362
C	50.713102	-42.714177	49.889415	C	50.708947	-42.851475	50.158071	C	50.683964	-43.088450	50.487067
C	49.993616	-44.055257	49.647349	C	50.020782	-44.219462	49.970507	C	50.047560	-44.487361	50.349141
C	50.000240	-41.933968	51.025524	C	50.017148	-42.064204	51.307256	C	49.999070	-42.312754	51.648925

C	48.499311	-41.612795	50.819532	C	48.504206	-41.773808	51.126851	C	48.468433	-42.089434	51.524757
O	47.867059	-41.338247	51.881908	O	47.896976	-41.488143	52.198895	O	47.899484	-41.779728	52.610879
O	48.030991	-41.621393	49.643797	O	48.012544	-41.817733	49.962659	O	47.927835	-42.203362	50.387571
C	50.854537	-41.858439	48.666832	C	50.776533	-42.034951	48.912421	C	50.664430	-42.292657	49.226908
C	52.192251	-41.549560	48.511396	C	52.099054	-41.684588	48.671286	C	51.955836	-41.880492	48.925997
N	55.069195	-40.775102	48.044284	N	54.926487	-40.820689	48.133500	N	54.702909	-40.854724	48.336563
C	53.959199	-40.202078	47.421596	C	53.803699	-40.305388	47.518979	C	53.545611	-40.423765	47.719896
C	54.385417	-39.137076	46.530517	C	54.176033	-39.220625	46.636709	C	53.842666	-39.325772	46.832093
C	55.738522	-39.053318	46.641233	C	55.530128	-39.054540	46.766439	C	55.184616	-39.068991	46.953942
C	56.152438	-40.069195	47.594326	C	55.989826	-40.048027	47.703329	C	55.716368	-40.024668	47.887467
N	57.051883	-42.173357	49.461620	N	56.966980	-42.220843	49.463769	N	56.859688	-42.162440	49.592187
C	57.881285	-41.246312	48.879956	C	57.770908	-41.227544	48.920835	C	57.596848	-41.134483	49.020571
C	59.264969	-41.548049	49.203130	C	59.154120	-41.532601	49.171355	C	59.002491	-41.404328	49.173551
C	59.252970	-42.687649	49.955006	C	59.182629	-42.739287	49.830871	C	59.108817	-42.627165	49.791395
C	57.863190	-43.055934	50.137471	C	57.812802	-43.137050	50.039385	C	57.766519	-43.075198	50.075350
N	55.103129	-43.569421	48.167302	N	54.985570	-43.607112	48.211478	N	54.987257	-43.728199	48.313606
O	55.842477	-43.593662	47.081806	O	55.724970	-43.626714	47.131384	O	55.493230	-43.529233	47.088343
O	54.378795	-44.693679	48.265143	O	54.226540	-44.712539	48.276967	O	54.237535	-44.877437	48.333642
C	52.817850	-39.154270	50.828390	C	52.817850	-39.154270	50.828390	C	52.817850	-39.154270	50.828390
C	53.561059	-40.165437	51.697435	C	53.534720	-40.139228	51.748155	C	53.388720	-40.136125	51.846632
S	55.210519	-40.601629	51.035260	S	55.172709	-40.679915	51.131776	S	55.000935	-40.866981	51.398113
H	54.550444	-45.658966	46.837255	H	54.502218	-45.677222	46.807281	H	54.471937	-45.741857	46.853850
H	49.308753	-52.419889	49.539555	H	49.306214	-52.410876	49.545538	H	49.308535	-52.399503	49.586869
H	50.986559	-52.615170	50.082033	H	50.991691	-52.652279	50.043416	H	51.015025	-52.702650	49.963391
H	50.639461	-52.257750	48.376096	H	50.614669	-52.219239	48.361875	H	50.546149	-52.160633	48.337872
H	49.718636	-50.001548	49.034285	H	49.743205	-49.979499	49.133063	H	49.776226	-49.956091	49.292579
H	50.053331	-50.352075	50.735223	H	50.108762	-50.407133	50.810301	H	50.232326	-50.490515	50.915880
H	52.494423	-50.472500	50.250960	H	52.539824	-50.548028	50.259136	H	52.620761	-50.640407	50.214167
H	52.168363	-50.181379	48.522620	H	52.171865	-50.167702	48.556772	H	52.161192	-50.169692	48.557430
H	54.864681	-47.634486	49.174031	H	54.879790	-47.651811	49.135461	H	54.945709	-47.729285	49.098597
H	54.144076	-49.218033	49.128356	H	54.151998	-49.232683	49.050776	H	54.173330	-49.284604	48.934670
H	53.438973	-45.729988	49.530962	H	53.444912	-45.760604	49.593194	H	53.542928	-45.832937	49.642228
H	51.858743	-46.010562	50.162857	H	51.927329	-46.089992	50.349971	H	52.116343	-46.187117	50.569061
H	51.965546	-46.308990	41.708596	H	51.932138	-46.336563	41.694323	H	51.917923	-46.361498	41.676688
H	51.550765	-46.943060	43.315075	H	51.578485	-46.924725	43.332097	H	51.592777	-46.899814	43.337942
H	53.854525	-45.974346	43.362127	H	53.864482	-45.948251	43.311513	H	53.878580	-45.940160	43.279055
H	54.352525	-46.980906	42.006240	H	54.333677	-46.933461	41.932209	H	54.322851	-46.925005	41.892136
H	54.154699	-49.023242	43.317095	H	54.266450	-48.980173	43.228249	H	54.315314	-48.964061	43.188883
H	53.285484	-48.211945	44.605232	H	53.363839	-48.234121	44.532093	H	53.397888	-48.244307	44.496236
H	53.526651	-46.536764	45.707301	H	53.525353	-46.578739	45.662949	H	53.521389	-46.641099	45.675556
H	57.461103	-47.454136	45.814997	H	57.495551	-47.320205	45.766544	H	57.507974	-47.261978	45.732372
H	56.753430	-46.542724	47.104572	H	56.738383	-46.470381	47.073345	H	56.740090	-46.472256	47.071191
H	57.670745	-45.143952	41.416012	H	57.730661	-45.143173	41.420072	H	57.809142	-45.143142	41.430641
H	56.722941	-45.416481	42.894365	H	56.696255	-45.407566	42.840730	H	56.666540	-45.396033	42.768717
H	58.498223	-45.400341	42.961782	H	58.464976	-45.409161	43.011305	H	58.416851	-45.420606	43.073162
H	58.497906	-42.933497	42.359682	H	58.516751	-42.938812	42.399865	H	58.547440	-42.953296	42.469494
H	56.746549	-42.963830	42.191453	H	56.773480	-42.959081	42.156573	H	56.826215	-42.950395	42.096545
H	56.517586	-43.554346	44.622891	H	56.452202	-43.566810	44.585406	H	56.309018	-43.527908	44.496268
H	57.253905	-41.967697	44.338012	H	57.162823	-41.966315	44.312888	H	57.068647	-41.947658	44.262582
H	59.532402	-43.046522	44.769642	H	59.449079	-42.994699	44.832549	H	59.294451	-43.014364	44.951953
H	58.678111	-44.552634	45.185121	H	58.605219	-44.503840	45.259299	H	58.386789	-44.495664	45.345598
H	58.344168	-41.934748	46.556298	H	58.167704	-41.856591	46.541452	H	57.918680	-41.825827	46.553432
H	59.065200	-43.276872	47.178312	H	58.917911	-43.143144	47.230749	H	58.607518	-43.108872	47.304960
H	51.698480	-43.468859	40.095591	H	51.745870	-43.453308	40.075586	H	51.919760	-43.378964	40.017463
H	52.435935	-41.912467	40.533594	H	52.409279	-41.879778	40.567530	H	52.291405	-41.776586	40.689393
H	50.849352	-42.360171	41.191379	H	50.828243	-42.407323	41.177959	H	50.769760	-42.586257	41.113270
H	53.507175	-43.797758	41.773889	H	53.530202	-43.748585	41.789054	H	53.591405	-43.569766	41.854244
H	51.957760	-44.288993	42.443753	H	51.987157	-44.318968	42.410165	H	52.109155	-44.411765	42.279689

H	51.846427	-42.456160	43.937423	H	51.760253	-42.515540	43.933698	H	51.474500	-42.771221	43.898829
H	52.967021	-41.465695	42.989851	H	52.873066	-41.470435	43.036964	H	52.577436	-41.551401	43.239471
H	54.864797	-42.807410	43.595136	H	54.794769	-42.779465	43.657562	H	54.535593	-42.805895	43.915660
H	53.855196	-44.116378	44.237147	H	53.801513	-44.111068	44.279207	H	53.574848	-44.218603	44.377123
H	53.939852	-41.439073	45.499953	H	53.846764	-41.428825	45.547448	H	53.335040	-41.620590	45.772854
H	54.849620	-42.774321	46.007520	H	54.723843	-42.774303	46.069539	H	54.358308	-42.903374	46.266185
H	58.171913	-44.658178	51.517083	H	58.203719	-44.823378	51.308895	H	58.286140	-44.800985	51.242008
H	51.791908	-44.124194	51.935805	H	51.901442	-44.134359	52.224182	H	52.012463	-44.310635	52.498395
H	51.897856	-40.069134	46.997848	H	51.717908	-40.275802	47.122291	H	51.451501	-40.522912	47.362354
H	58.226882	-39.574541	47.602292	H	58.041083	-39.485493	47.726260	H	57.738952	-39.370872	47.837313
H	57.133045	-46.783820	52.174726	H	57.079302	-46.999902	51.994750	H	57.230815	-47.054157	51.918425
H	55.500561	-46.990718	51.440328	H	55.387350	-47.100306	51.388555	H	55.511507	-47.160351	51.393563
H	55.738795	-47.215390	53.186605	H	55.747376	-47.392131	53.105204	H	55.962246	-47.503730	53.080445
H	56.294350	-43.558330	53.974671	H	56.532701	-43.795804	53.956066	H	56.730629	-43.921083	54.006651
H	55.858428	-45.081090	54.728420	H	56.111262	-45.337049	54.684886	H	56.416573	-45.504144	54.696679
H	53.623286	-45.370568	53.354749	H	53.756710	-45.458524	53.477350	H	53.973386	-45.617237	53.636553
H	50.498631	-44.645395	48.870855	H	50.508525	-44.803331	49.177725	H	50.522031	-45.061696	49.541754
H	48.962681	-43.863255	49.329572	H	48.974045	-44.057584	49.691448	H	48.983314	-44.372657	50.117424
H	49.965027	-44.641632	50.578496	H	50.042714	-44.792248	50.909237	H	50.138101	-45.045112	51.292444
H	50.520502	-40.976918	51.178415	H	50.521874	-41.094625	51.430812	H	50.462533	-41.318956	51.738981
H	50.111725	-42.497456	51.963649	H	50.155392	-42.609901	52.250903	H	50.197266	-42.836016	52.594668
H	50.021852	-41.373685	48.169493	H	49.903314	-41.632991	48.410418	H	49.753992	-41.952722	48.745560
H	53.711239	-38.528778	45.934991	H	53.475908	-38.640526	46.042281	H	53.105315	-38.800052	46.232139
H	56.416096	-38.360583	46.150586	H	56.168865	-38.319126	46.285522	H	55.770642	-38.299012	46.460346
H	60.116982	-40.953100	48.886599	H	59.990418	-40.909929	48.865809	H	59.799186	-40.752239	48.826704
H	60.090701	-43.217806	50.397870	H	60.043915	-43.284128	50.205851	H	60.008301	-43.159318	50.086318
H	52.660529	-39.538055	49.818193	H	52.612243	-39.595674	49.850817	H	52.566650	-39.647853	49.889293
H	52.976240	-41.083512	51.826381	H	52.913757	-41.021389	51.940968	H	52.689142	-40.958894	52.041836
H	53.740204	-39.750649	52.699720	H	53.736469	-39.672769	52.723225	H	53.577330	-39.636161	52.806781
H	50.919510	-48.109600	50.045022	H	51.001763	-48.165729	50.240340	H	51.122710	-48.225736	50.370952
H	56.151974	-48.392033	44.238377	H	56.233711	-48.275665	44.158664	H	56.273780	-48.194800	44.100137
H	57.382346	-43.248769	46.886989	H	57.251743	-43.195989	46.902995	H	56.929780	-43.160657	46.885951
H	53.178544	-42.865774	46.034254	H	53.054051	-42.841431	46.058696	H	52.684345	-43.122852	46.212748
H	51.832975	-38.919402	51.261771	H	51.860395	-38.839280	51.271972	H	51.901564	-38.696914	51.229288
H	53.388432	-38.218725	50.749890	H	53.433333	-38.258438	50.668378	H	53.536003	-38.352084	50.612304
O	52.127757	-43.992763	46.817677	O	52.010161	-44.066442	46.823195	O	51.864748	-44.395777	47.157930
H	52.779209	-44.255700	47.517422	H	52.706102	-44.337940	47.480178	H	52.685139	-44.579085	47.707194
H	51.539605	-43.344250	47.284019	H	51.416210	-43.483406	47.351112	H	51.313525	-43.822356	47.736319
O	56.288666	-46.409051	48.902583	O	56.237660	-46.382777	48.842742	O	56.299980	-46.426704	48.828142
H	55.611583	-45.685100	48.759980	H	55.517812	-45.707072	48.695459	H	55.533218	-45.783347	48.708168
H	56.857868	-46.062430	49.619500	H	56.795048	-45.955816	49.534265	H	56.858378	-45.982876	49.505101
H	52.022267	-48.052608	42.009103	H	52.018957	-48.067415	42.046930	H	52.011815	-48.078877	42.079910

Heme (Fe³⁺) with NO₂⁻

S=1/2			S=3/2			S=5/2					
C	50.331000	-52.045950	49.409000	C	50.331000	-52.045950	49.409000	C	50.331000	-52.045950	49.409000
C	50.439999	-50.558739	49.744984	C	50.500108	-50.596924	49.865194	C	50.502266	-50.643529	49.993159
C	51.861528	-50.029592	49.568927	C	51.903755	-50.065466	49.585741	C	51.840363	-50.027706	49.594955
N	51.896360	-48.594182	49.857614	N	51.993067	-48.662315	49.995995	N	51.948859	-48.659724	50.106084
C	52.943831	-47.789846	49.652055	C	53.040785	-47.860527	49.789220	C	53.001219	-47.859908	49.909246
N	54.085757	-48.278174	49.149078	N	54.114767	-48.302525	49.119596	N	54.038090	-48.280541	49.175454
N	52.851802	-46.487356	49.948206	N	53.023509	-46.603305	50.254486	N	53.042537	-46.634775	50.458446
C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410
C	53.691265	-46.960458	42.865852	C	53.694158	-46.906269	42.837185	C	53.703258	-46.965961	42.824989
C	54.074547	-48.084486	43.833581	C	54.134265	-48.012742	43.800499	C	54.098069	-48.055457	43.829501
N	55.357057	-47.878291	44.504812	N	55.412655	-47.750799	44.460286	N	55.347536	-47.782812	44.535151
C	55.531176	-47.050338	45.542326	C	55.557472	-46.947697	45.520123	C	55.451371	-46.982927	45.604956
N	54.497962	-46.365686	46.037896	N	54.495095	-46.332254	46.049017	N	54.360830	-46.449013	46.159837
N	56.758066	-46.864541	46.067308	N	56.779411	-46.708962	46.035958	N	56.663870	-46.678123	46.108969

C	57.624000	-44.932480	42.491060	C	57.624000	-44.932480	42.491060	C	57.624000	-44.932480	42.491060
C	57.584000	-43.404240	42.750400	C	57.584000	-43.404240	42.750400	C	57.584000	-43.404240	42.750400
C	57.424555	-43.049750	44.234551	C	57.261075	-43.021825	44.202895	C	57.090061	-42.998538	44.144993
C	58.604865	-43.451968	45.109126	C	58.368727	-43.330065	45.203787	C	58.034479	-43.398343	45.272805
N	58.398795	-42.923963	46.497302	N	58.053344	-42.688443	46.523531	N	57.623733	-42.741809	46.553940
C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430
C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930
C	52.774138	-42.485546	43.301301	C	52.474468	-42.605498	43.406129	C	52.215457	-42.830736	43.483008
C	53.934570	-43.038231	44.107277	C	53.623784	-43.044907	44.290382	C	53.017334	-43.610992	44.509204
N	54.016693	-42.434064	45.460454	N	53.501369	-42.526540	45.673561	N	52.894823	-43.080930	45.890785
Fe	55.036194	-42.215933	49.480811	Fe	54.884061	-42.264438	49.738644	Fe	54.741493	-42.293682	49.881062
C	57.575767	-43.967806	50.908917	C	57.527664	-44.116283	50.802621	C	57.488770	-44.101888	50.767829
C	52.749701	-43.736301	51.500739	C	52.793405	-43.862754	51.867118	C	52.858787	-43.830447	52.189291
C	52.526055	-40.717007	47.697511	C	52.244265	-40.993317	47.985169	C	52.014649	-41.269953	48.141810
C	57.320597	-40.134118	47.967136	C	56.983560	-39.988030	48.302268	C	56.682856	-39.965351	48.353853
N	55.169551	-43.587848	50.941973	N	55.144134	-43.732511	51.092490	N	55.125627	-43.749101	51.218628
C	56.285285	-44.203074	51.378849	C	56.300130	-44.363665	51.396727	C	56.308443	-44.388024	51.424196
C	56.007164	-45.122398	52.561084	C	56.126043	-45.302101	52.592090	C	56.218430	-45.337142	52.624491
C	56.365066	-46.603804	52.305047	C	56.373391	-46.789879	52.257096	C	56.339669	-46.832285	52.244020
C	56.677700	-44.591925	53.877229	C	56.984231	-44.831653	53.809941	C	57.225739	-44.958959	53.753765
C	58.206986	-44.809064	54.103136	C	58.531587	-45.023839	53.789426	C	58.728038	-45.322618	53.599588
O	58.923181	-45.305998	53.188440	O	59.081369	-45.667118	52.849271	O	59.160081	-45.847404	52.531720
O	58.579306	-44.441113	55.248474	O	59.101705	-44.499807	54.784083	O	59.416345	-45.040502	54.618560
C	54.545407	-44.934309	52.697687	C	54.691890	-45.063549	52.906060	C	54.830864	-45.045105	53.083757
C	54.097087	-44.049694	51.741964	C	54.158055	-44.166664	51.998646	C	54.231980	-44.151944	52.218267
N	53.056435	-42.300058	49.556118	N	52.904907	-42.464804	49.873278	N	52.828328	-42.555075	50.104676
C	52.288037	-42.997351	50.444888	C	52.230893	-43.181078	50.811353	C	52.221998	-43.200239	51.153601
C	50.797234	-42.849177	50.156905	C	50.726347	-43.159307	50.566079	C	50.704259	-43.187911	51.015825
C	50.100609	-44.207973	49.939530	C	50.126692	-44.575682	50.451628	C	50.084811	-44.596246	51.102310
C	50.114988	-42.082025	51.330949	C	50.032123	-42.380460	51.724921	C	50.117293	-42.273659	52.136984
C	48.602247	-41.787128	51.147373	C	48.493974	-42.201034	51.591884	C	48.582245	-42.081981	52.110211
O	47.988253	-41.563769	52.226960	O	47.920936	-41.907056	52.677138	O	48.093058	-41.692470	53.208890
O	48.132832	-41.768248	49.974452	O	47.966637	-42.331395	50.452255	O	47.955055	-42.289319	51.036020
C	50.843967	-41.999196	48.939775	C	50.670247	-42.378632	49.299020	C	50.556705	-42.546938	49.678973
C	52.153477	-41.665269	48.675794	C	51.946180	-41.933446	48.985765	C	51.799593	-42.126563	49.233378
N	54.950634	-40.769625	48.088511	N	54.662383	-40.809447	48.395319	N	54.415226	-40.927338	48.501938
C	53.799709	-40.272578	47.478456	C	53.485391	-40.419256	47.783068	C	53.225883	-40.660542	47.856210
C	54.147098	-39.210320	46.550251	C	53.736105	-39.288930	46.918468	C	53.402894	-39.556778	46.944588
C	55.494632	-39.050316	46.629694	C	55.060620	-38.972243	47.053993	C	54.694203	-39.124447	47.087000
C	55.983627	-40.019390	47.596241	C	55.636521	-39.927183	47.965641	C	55.332378	-39.988451	48.042382
N	57.035442	-42.074309	49.436881	N	56.862241	-42.080700	49.581921	N	56.713095	-42.066135	49.612740
C	57.801092	-41.103676	48.832632	C	57.561892	-41.018284	49.032489	C	57.347267	-40.966471	49.060041
C	59.208387	-41.333987	49.112693	C	58.976765	-41.254525	49.166860	C	58.768755	-41.164193	49.103876
C	59.280031	-42.477358	49.849833	C	59.124359	-42.488783	49.748867	C	58.981696	-42.415391	49.639605
C	57.916978	-42.920411	50.075024	C	57.797626	-42.979344	50.037609	C	57.690189	-42.950013	49.987014
N	55.112747	-43.564791	48.201705	N	54.930087	-43.602854	48.366178	N	54.904507	-43.765472	48.459792
O	55.862329	-43.577903	47.141654	O	55.542269	-43.465011	47.240810	O	55.174350	-43.473244	47.195601
O	54.396686	-44.681940	48.306881	O	54.322385	-44.762596	48.479804	O	54.185570	-44.911339	48.560686
C	52.817850	-39.154270	50.828390	C	52.817850	-39.154270	50.828390	C	52.817850	-39.154270	50.828390
C	53.579354	-40.113204	51.736889	C	53.410708	-40.102515	51.866127	C	53.418789	-40.007583	51.942238
S	55.218772	-40.594923	51.084525	S	55.003329	-40.875733	51.436240	S	54.978862	-40.849550	51.524610
H	54.606987	-45.704785	46.828355	H	54.583846	-45.711311	46.867177	H	54.411783	-45.824920	46.988162
H	49.301982	-52.397813	49.547044	H	49.316175	-52.401304	49.622646	H	49.366922	-52.474465	49.706427
H	50.982375	-52.648899	50.055931	H	51.036222	-52.710951	49.925850	H	51.122055	-52.721470	49.760811
H	50.616674	-52.239128	48.366001	H	50.502008	-52.144801	48.328184	H	50.366527	-52.024727	48.311521
H	49.765486	-49.978520	49.097750	H	49.770702	-49.954174	49.349707	H	49.690517	-49.989991	49.639576
H	50.121221	-50.383258	50.783163	H	50.297533	-50.514948	50.943434	H	50.435039	-50.678404	51.090310
H	52.552255	-50.561515	50.241345	H	52.653376	-50.660018	50.130889	H	52.669754	-50.631435	49.995279

H	52.194096	-50.197739	48.532674	H	52.120864	-50.142928	48.508602	H	51.926371	-50.015037	48.495801
H	54.940252	-47.706476	49.149953	H	54.988387	-47.762670	49.131241	H	54.926135	-47.763030	49.179010
H	54.195792	-49.279670	49.052402	H	54.174432	-49.280999	48.867445	H	54.026937	-49.207063	48.770636
H	53.530771	-45.803453	49.603844	H	53.634574	-45.884036	49.857390	H	53.588111	-45.893335	49.991603
H	51.980233	-46.104648	50.295798	H	52.204882	-46.256795	50.741533	H	52.263362	-46.321202	51.026060
H	51.972592	-46.326719	41.689614	H	51.936752	-46.364091	41.667285	H	51.968093	-46.396635	41.628886
H	51.559977	-46.909788	43.315303	H	51.569206	-46.900953	43.320589	H	51.582801	-46.819125	43.311554
H	53.874701	-45.988783	43.345534	H	53.853973	-45.927620	43.310859	H	53.920561	-45.981601	43.261128
H	54.349627	-47.002212	41.987464	H	54.336436	-46.928311	41.946317	H	54.335889	-47.054811	41.931655
H	54.144403	-49.039534	43.302501	H	54.240463	-48.964628	43.269498	H	54.219567	-49.020384	43.325680
H	53.291581	-48.221345	44.596286	H	53.365421	-48.183878	44.570210	H	53.297527	-48.207965	44.569168
H	53.556617	-46.577951	45.733230	H	53.560272	-46.608358	45.775907	H	53.446844	-46.793170	45.894980
H	57.500414	-47.477159	45.747327	H	57.547504	-47.270425	45.683094	H	57.458798	-47.183001	45.731025
H	56.803563	-46.595004	47.062074	H	56.818947	-46.499737	47.048096	H	56.703196	-46.495379	47.129070
H	57.669193	-45.142164	41.415866	H	57.813383	-45.140056	41.431435	H	57.920187	-45.140817	41.456774
H	56.723250	-45.417223	42.894250	H	56.664675	-45.395486	42.762119	H	56.634202	-45.379835	42.658720
H	58.499374	-45.400533	42.959305	H	58.414286	-45.422308	43.075062	H	58.340398	-45.437507	43.152177
H	58.494345	-42.931821	42.354211	H	58.541621	-42.949625	42.457895	H	58.583658	-42.976726	42.583953
H	56.743026	-42.964494	42.196423	H	56.818274	-42.954160	42.103722	H	56.921713	-42.937241	42.008934
H	56.534277	-43.557519	44.632694	H	56.351990	-43.549213	44.527847	H	56.099675	-43.440193	44.334769
H	57.259906	-41.965539	44.335283	H	57.044251	-41.943223	44.245063	H	56.957832	-41.905922	44.167777
H	59.550599	-43.043429	44.737838	H	59.335496	-42.935011	44.874139	H	59.063445	-43.090470	45.055607
H	58.698353	-44.539254	45.194332	H	58.469637	-44.403756	45.389607	H	58.019731	-44.477883	45.454173
H	58.403811	-41.894168	46.512111	H	58.007489	-41.664981	46.438593	H	57.613438	-41.719642	46.457575
H	59.129870	-43.226011	47.152762	H	58.760652	-42.879762	47.249949	H	58.275651	-42.945916	47.326993
H	51.681203	-43.474618	40.104067	H	51.900890	-43.389471	40.023911	H	52.123881	-43.250694	39.980686
H	52.445596	-41.925738	40.520438	H	52.306599	-41.787520	40.675661	H	52.112454	-41.691682	40.829390
H	50.857613	-42.342922	41.195606	H	50.774947	-42.566394	41.121255	H	50.744920	-42.808686	41.006822
H	53.498637	-43.815059	41.769674	H	53.586203	-43.588672	41.846771	H	53.621312	-43.371297	41.959111
H	51.947525	-44.277356	42.456878	H	52.094818	-44.402067	42.297708	H	52.269729	-44.478396	42.122999
H	51.870165	-42.414954	43.923557	H	51.512261	-42.758685	43.915764	H	51.139514	-42.899753	43.702906
H	53.017589	-41.467332	42.963699	H	52.567366	-41.528627	43.200878	H	52.495062	-41.766505	43.526006
H	54.878528	-42.859397	43.585674	H	54.573008	-42.692126	43.877076	H	54.081879	-43.589120	44.243985
H	53.828655	-44.118801	44.266358	H	53.672306	-44.137957	44.373603	H	52.703298	-44.660584	44.534481
H	53.987892	-41.406625	45.441840	H	53.305367	-41.518845	45.706713	H	52.663223	-42.083111	45.905537
H	54.871564	-42.735369	45.990333	H	54.375080	-42.698415	46.224530	H	53.825016	-43.196537	46.415413
H	58.369805	-44.531504	51.403715	H	58.368364	-44.705873	51.172250	H	58.362611	-44.676699	51.083762
H	52.020459	-44.176405	52.178274	H	52.124020	-44.304996	52.602802	H	52.245766	-44.247936	52.985739
H	51.718289	-40.260321	47.128328	H	51.404205	-40.606570	47.410629	H	51.134909	-40.947948	47.587343
H	58.029992	-39.426528	47.541422	H	57.637862	-39.209153	47.913356	H	57.283135	-39.162997	47.927180
H	57.440538	-46.702096	52.128430	H	57.418670	-46.932890	51.965246	H	57.333711	-47.028867	51.829828
H	55.794700	-46.999978	51.456097	H	55.697359	-47.125343	51.461647	H	55.557703	-47.113310	51.530020
H	56.108270	-47.193219	53.194151	H	56.180239	-47.397545	53.150558	H	56.216421	-47.442754	53.147928
H	56.483892	-43.514086	53.966322	H	56.788988	-43.766029	53.988615	H	57.167489	-43.877242	53.937631
H	56.165229	-45.070108	54.722920	H	56.617688	-45.365252	54.699360	H	56.881936	-45.444580	54.678343
H	53.923490	-45.434894	53.434143	H	54.141063	-45.564136	53.696861	H	54.344035	-45.534111	53.922400
H	50.577919	-44.777027	49.129838	H	50.609272	-45.146929	49.646662	H	50.493747	-45.253159	50.322186
H	49.052401	-44.035778	49.674468	H	49.058651	-44.490263	50.226209	H	49.002607	-44.519944	50.954712
H	50.129269	-44.799277	50.865723	H	50.236844	-45.117982	51.401458	H	50.271430	-45.043899	52.087391
H	50.620551	-41.115984	51.473406	H	50.468733	-41.373453	51.796258	H	50.566524	-41.272858	52.059086
H	50.258791	-42.653943	52.257498	H	50.246737	-42.887008	52.675483	H	50.409661	-42.679241	53.114906
H	49.961189	-41.618901	48.437490	H	49.743383	-42.076782	48.823997	H	49.599153	-42.303268	49.232489
H	53.428562	-38.651972	45.958249	H	52.976103	-38.781352	46.331910	H	52.616755	-39.139560	46.322780
H	56.123264	-38.335458	46.107672	H	55.611558	-38.164956	46.581054	H	55.186447	-38.298484	46.582603
H	60.016546	-40.692296	48.774558	H	59.751474	-40.569046	48.836032	H	59.505264	-40.452608	48.743411
H	60.157293	-42.968460	50.259116	H	60.040899	-42.999814	50.026789	H	59.926019	-42.909978	49.843693
H	52.612960	-39.596355	49.852282	H	52.454199	-39.687500	49.950251	H	52.375886	-39.768958	50.043762
H	52.995392	-41.016248	51.946149	H	52.712002	-40.914367	52.110853	H	52.709926	-40.769683	52.290851

H	53.789290	-39.638651	52.705528	H	53.629840	-39.570150	52.801586	H	53.684060	-39.389893	52.810424
H	51.037113	-48.166343	50.187340	H	51.175794	-48.255952	50.440135	H	51.130287	-48.258290	50.552236
H	56.155155	-48.422887	44.198477	H	56.236265	-48.237902	44.125060	H	56.201220	-48.194238	44.174551
H	57.453162	-43.200854	46.894259	H	57.115371	-42.987912	46.909089	H	56.627068	-43.032973	46.870919
H	53.207233	-42.803383	46.027503	H	52.746364	-43.048148	46.193819	H	52.189303	-43.609936	46.462212
H	51.855678	-38.875880	51.284172	H	51.969424	-38.618105	51.275752	H	52.024956	-38.519649	51.246997
H	53.396553	-38.235604	50.664891	H	53.557899	-38.412296	50.501629	H	53.575018	-38.502937	50.374619
O	52.196032	-44.042070	46.797729	O	51.937446	-44.345285	47.104763	O	51.634426	-44.814785	47.649765
H	52.846394	-44.298327	47.501161	H	52.667771	-44.548813	47.739372	H	52.525211	-44.840870	48.104042
H	51.523090	-43.513174	47.274217	H	51.293883	-43.839773	47.650115	H	51.080624	-44.255230	48.235245
O	56.333440	-46.441592	48.874364	O	56.379126	-46.455016	48.842839	O	56.292552	-46.487790	48.890161
H	55.685374	-45.693017	48.771758	H	55.690069	-45.741382	48.804551	H	55.554134	-45.811593	48.870298
H	56.957727	-46.141819	49.563348	H	57.015476	-46.128211	49.511590	H	56.924887	-46.136266	49.548378
H	52.003573	-48.060118	42.038211	H	52.026718	-48.080013	42.075419	H	51.969671	-48.087486	42.134475

Table S9. Cartesian coordinates (Å) of the heme species (Fe²⁺ & Fe³⁺) without ligands (and without the cubane cluster) optimized at DFT (BP86 functional) using TZ2P basis sets. S is the spin state of the species.

			Heme (Fe ²⁺) without HSO ₃ ⁻								
			S=0		S=1		S=2				
C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000
C	51.626816	5.182187	71.437405	C	51.588097	5.069956	71.070520	C	51.580616	5.263094	71.474370
C	51.772848	5.647207	69.993800	C	51.287329	6.032242	69.920435	C	51.676542	5.903988	70.089894
N	52.978464	6.459853	69.825150	N	52.545891	6.583883	69.399929	N	52.951126	6.615875	69.962272
C	53.332775	7.027386	68.670520	C	52.664370	7.455007	68.395130	C	53.285345	7.462604	68.986611
N	52.581683	6.836652	67.579579	N	51.577697	7.985160	67.824721	N	52.404950	7.774289	68.018095
N	54.471418	7.739947	68.568328	N	53.879813	7.764286	67.901618	N	54.525714	7.961657	68.922587
C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000
C	53.680222	2.637733	63.629170	C	53.655574	2.787987	63.465244	C	53.725261	2.554480	63.388836
C	53.901256	2.944746	65.113003	C	54.239472	2.570752	64.865236	C	54.318248	2.306377	64.783274
N	55.263940	3.389140	65.415247	N	55.542764	3.220020	65.042339	N	55.628953	2.931613	64.973112
C	55.731879	4.615086	65.176070	C	55.703618	4.547029	65.131109	C	55.799764	4.253411	65.134163
N	54.900952	5.614532	64.861112	N	54.662561	5.343757	65.380096	N	54.747541	5.034349	65.380792
N	57.053594	4.860191	65.213917	N	56.917429	5.093908	64.958525	N	57.026151	4.783922	65.049226
C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000
C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000
C	57.546480	6.216792	61.411813	C	57.741978	6.218880	61.415074	C	57.928155	6.187157	61.405760
C	58.754604	6.485251	62.306183	C	59.164810	6.429887	61.918150	C	59.412682	6.254296	61.744727
N	58.630723	7.825227	62.945432	N	59.310587	7.709286	62.681319	N	59.729588	7.400274	62.652796
C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000
C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000
C	52.580904	5.873555	60.498990	C	53.176638	5.734850	60.182371	C	52.695688	5.868375	60.497069
C	53.031713	6.187560	61.915299	C	53.794808	6.147266	61.504887	C	53.421235	6.110710	61.816033
N	53.104433	7.652271	62.195763	N	54.374937	7.524070	61.479720	N	53.421243	7.530372	62.265430
Fe	54.663781	10.703963	64.105321	Fe	55.467380	10.579920	62.761749	Fe	55.031214	10.438356	63.105735
C	58.051844	10.423960	64.172393	C	57.866723	10.741218	65.204047	C	57.974364	10.324821	64.887928
C	54.595342	10.632587	67.504130	C	53.024954	10.311904	65.155786	C	53.260394	10.392573	66.058715
C	51.217252	10.642192	64.021312	C	53.103095	10.187114	60.293828	C	52.099952	10.259905	61.306300
C	54.742525	10.665072	60.675155	C	57.947220	10.293717	60.351652	C	56.795534	9.936041	60.169610
N	55.987448	10.262463	65.466400	N	55.472933	10.469703	64.774961	N	55.549233	10.174303	65.124016
C	57.345589	10.040178	65.280233	C	56.565967	10.642770	65.613049	C	56.819961	10.282664	65.631876
C	57.968533	9.426091	66.523704	C	56.174350	10.732610	67.090376	C	56.824506	10.447372	67.151541
C	57.784370	7.871001	66.511588	C	56.744408	9.548260	67.906585	C	57.437193	9.210823	67.856779
C	59.445096	9.772008	66.751697	C	56.565523	12.092378	67.733699	C	57.526067	11.755357	67.621032
C	60.554894	9.087983	65.907942	C	58.037435	12.402353	68.132160	C	59.077581	11.825407	67.727151
O	60.261665	8.311794	64.919385	O	58.954080	11.556148	67.903785	O	59.795329	10.921819	67.198951
O	61.723062	9.336509	66.269301	O	58.180623	13.528132	68.683553	O	59.492629	12.836445	68.355545
C	56.986532	9.937366	67.545122	C	54.683490	10.644362	66.961905	C	55.349023	10.539922	67.402013
C	55.835731	10.290590	66.899346	C	54.336960	10.507747	65.648366	C	54.669346	10.392632	66.223900

N	53.207419	10.568591	65.491676	N	53.510119	10.266022	62.752184	N	53.126167	10.344923	63.596403
C	53.411016	10.767384	66.854177	C	52.674581	10.171063	63.849433	C	52.587124	10.385879	64.866902
C	52.120976	11.170393	67.569624	C	51.237315	9.833067	63.456609	C	51.058268	10.440258	64.842610
C	51.772174	10.253410	68.756287	C	50.936372	8.362906	63.854187	C	50.414109	9.298983	65.653778
C	52.270109	12.642480	68.055017	C	50.201450	10.794801	64.091912	C	50.583119	11.816198	65.396325
C	51.013018	13.290155	68.690230	C	48.764032	10.273900	63.861203	C	49.042465	11.972340	65.491798
O	51.248266	14.356334	69.327150	O	48.176310	9.781966	64.870327	O	48.627478	12.600609	66.507135
O	49.888977	12.738185	68.514123	O	48.320238	10.346247	62.679836	O	48.345041	11.483663	64.557222
C	51.143124	11.072087	66.447965	C	51.334995	9.946370	61.976575	C	50.806217	10.327003	63.382399
C	51.810487	10.785579	65.291410	C	52.650270	10.163895	61.622223	C	52.002873	10.310402	62.709843
N	53.318374	10.549118	62.701998	N	55.520188	10.235060	60.780537	N	54.542516	10.019517	61.166655
C	51.910189	10.483624	62.852029	C	54.429640	10.199820	59.913837	C	53.271231	10.133282	60.596824
C	51.280571	10.327433	61.561980	C	54.870107	10.069386	58.548934	C	53.359131	10.037323	59.163834
C	52.270897	10.353853	60.624496	C	56.234254	10.030852	58.571462	C	54.681255	9.888604	58.851721
C	53.525015	10.516524	61.320910	C	56.638959	10.159406	59.943793	C	55.416287	9.910486	60.086091
N	56.111359	10.603767	62.698979	N	57.472978	10.498982	62.772250	N	56.961116	10.174242	62.624769
C	55.962309	10.764919	61.321359	C	58.341039	10.500478	61.666737	C	57.511677	10.104855	61.345706
C	57.233891	11.004445	60.712648	C	59.685137	10.727145	62.092186	C	58.933305	10.255068	61.413379
C	58.168301	11.009634	61.724010	C	59.655095	10.849863	63.465334	C	59.255763	10.411706	62.747417
C	57.466468	10.746559	62.944841	C	58.292384	10.708774	63.866577	C	58.031862	10.324118	63.485539
C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000
C	53.265328	13.615013	64.094531	C	54.040743	13.423461	63.516107	C	53.867378	13.533259	63.737070
S	54.903912	12.839796	64.277417	S	55.437295	12.719691	62.569186	S	55.382749	12.703266	63.129396
H	55.243521	6.486079	64.441316	H	54.722032	6.347721	65.143408	H	54.784379	6.064945	65.310452
H	50.236187	4.048931	72.664627	H	50.593042	3.738124	72.466337	H	50.275796	3.977444	72.641331
H	50.301989	3.512429	70.975906	H	49.834729	3.784063	70.862136	H	50.338436	3.558445	70.916670
H	49.454731	5.015847	71.401100	H	49.607691	5.136558	71.993969	H	49.416956	4.978416	71.456828
H	51.632436	6.061266	72.098979	H	52.099041	5.627931	71.869741	H	51.585043	6.059435	72.232999
H	52.494565	4.563277	71.708635	H	52.292538	4.303088	70.712737	H	52.480420	4.651533	71.645208
H	51.827944	4.779722	69.318735	H	50.759541	5.512055	69.106769	H	51.601486	5.136614	69.302781
H	50.889136	6.243381	69.712503	H	50.644754	6.851888	70.276977	H	50.847601	6.614520	69.953940
H	52.816943	7.278989	66.680092	H	51.680168	8.628359	67.047918	H	52.598543	8.582149	67.420777
H	51.646183	6.461270	67.679394	H	50.660736	7.897780	68.245238	H	51.425149	7.548739	68.148968
H	54.466823	8.567106	67.951092	H	54.039747	8.694494	67.472544	H	54.740890	8.762262	68.306205
H	55.006747	7.881185	69.419347	H	54.689193	7.393498	68.388240	H	55.166720	7.801031	69.691293
H	52.090562	1.981793	62.296830	H	51.845403	2.395763	62.326697	H	51.837176	2.327516	62.324223
H	51.548055	3.107095	63.560689	H	51.550700	2.804100	64.027470	H	51.665664	2.981628	63.966836
H	53.975010	3.511501	63.029332	H	53.674583	3.862991	63.236987	H	53.914111	3.599012	63.105049
H	54.349189	1.817150	63.335629	H	54.310354	2.297334	62.731125	H	54.261816	1.934449	62.658124
H	53.721114	2.052737	65.722812	H	54.389329	1.504593	65.064858	H	54.447638	1.234965	64.968364
H	53.184480	3.699424	65.468982	H	53.546924	2.927887	65.641966	H	53.633821	2.660922	65.568849
H	53.904477	5.519390	65.004528	H	53.743554	4.939967	65.504998	H	53.835565	4.611816	65.492705
H	57.690920	4.102515	65.432279	H	57.714317	4.490746	64.800013	H	57.806900	4.196399	64.788649
H	57.367588	5.793280	65.475092	H	57.112085	6.069091	65.209133	H	57.223601	5.777410	65.209004
H	57.573691	2.708443	61.203841	H	57.522345	2.710841	61.208181	H	57.435660	2.714629	61.223970
H	56.770518	3.716116	62.424871	H	56.794657	3.746604	62.448811	H	56.847976	3.798015	62.498093
H	58.544475	3.669583	62.329682	H	58.566086	3.636447	62.295088	H	58.596672	3.583590	62.234759
H	58.458423	4.792753	60.064078	H	58.369315	4.727047	59.969924	H	58.277562	4.663492	59.896592
H	56.697822	4.752441	60.086747	H	56.628186	4.829668	60.187622	H	56.580728	4.916663	60.287800
H	56.635614	6.287998	62.028237	H	57.043282	6.288960	62.265978	H	57.334462	6.290553	62.329099
H	57.477665	7.011084	60.652973	H	57.497782	7.029397	60.709987	H	57.660535	7.035423	60.760168
H	59.694038	6.461180	61.743704	H	59.866264	6.470233	61.078546	H	60.017909	6.374594	60.839801
H	58.825599	5.751839	63.116428	H	59.483262	5.626319	62.589652	H	59.750209	5.349924	62.261085
H	58.732330	8.580521	62.255376	H	58.963248	8.532895	62.145597	H	59.465989	8.325904	62.243859
H	59.324478	8.032660	63.768360	H	60.297075	7.906704	62.877120	H	60.734523	7.446224	62.850503
H	51.834025	2.765633	59.011117	H	51.391084	2.872730	59.206198	H	51.766029	2.767513	59.054059
H	52.348783	4.228996	58.148160	H	52.550914	3.783775	58.217169	H	52.392616	4.161829	58.149501
H	50.795997	4.207342	59.010215	H	51.038183	4.550342	58.745392	H	50.820644	4.268326	58.967510

H	53.556099	3.955060	60.368703	H	53.301235	3.628316	60.627410	H	53.525159	3.883535	60.393983
H	52.001414	3.929861	61.190976	H	51.798246	4.394623	61.145822	H	51.963240	3.988189	61.192022
H	51.582874	6.307621	60.333137	H	52.418227	6.476334	59.888009	H	51.709170	6.355571	60.521284
H	53.263312	6.330832	59.767459	H	53.943203	5.722372	59.392929	H	53.258746	6.310600	59.662711
H	54.027257	5.776144	62.122978	H	54.601332	5.466598	61.806044	H	54.469600	5.794909	61.757626
H	52.328376	5.764736	62.642197	H	53.040442	6.149818	62.301378	H	52.938945	5.539329	62.617709
H	53.925016	8.091653	61.763417	H	55.220632	7.597846	60.903101	H	53.997092	8.177137	61.681980
H	53.133339	7.839394	63.234673	H	54.607374	7.811959	62.464665	H	53.790666	7.615316	63.249196
H	59.136322	10.372591	64.210651	H	58.603844	10.934970	65.987407	H	58.897647	10.485986	65.451680
H	54.616921	10.826189	68.575799	H	52.221774	10.324310	65.892059	H	52.671819	10.584983	66.956455
H	50.130809	10.682821	63.966965	H	52.347841	10.136113	59.512185	H	51.166700	10.310522	60.748806
H	54.731579	10.714615	59.587962	H	58.722706	10.276221	59.587086	H	57.358377	9.880285	59.239286
H	58.405380	7.419939	65.726805	H	57.832992	9.645908	67.984382	H	58.510240	9.164085	67.642697
H	56.719579	7.623492	66.394122	H	56.491794	8.591434	67.427801	H	56.941063	8.287433	67.528769
H	58.111362	7.465590	67.477288	H	56.322091	9.560436	68.921175	H	57.314180	9.312387	68.943645
H	59.587177	10.857118	66.646219	H	56.232073	12.902484	67.070155	H	57.208835	12.580929	66.967292
H	59.693912	9.543279	67.797543	H	55.974300	12.200156	68.655833	H	57.138118	11.997782	68.620436
H	57.090294	9.803472	68.618602	H	53.985003	10.824092	67.776389	H	54.904814	10.840459	68.348162
H	51.632280	9.218655	68.419470	H	51.718073	7.691072	63.470152	H	50.837840	8.324662	65.373232
H	50.843011	10.604095	69.217808	H	49.976107	8.041711	63.435705	H	49.335470	9.282764	65.462770
H	52.572278	10.277129	69.508093	H	50.883565	8.257453	64.945637	H	50.560481	9.466303	66.730022
H	52.573386	13.271462	67.205035	H	50.325590	11.790144	63.645701	H	50.965324	12.615152	64.744243
H	53.096204	12.687131	68.779490	H	50.387774	10.869367	65.170745	H	51.021224	11.970858	66.391134
H	50.084389	11.278984	66.551738	H	50.495565	9.837228	61.298738	H	49.817437	10.347710	62.939775
H	50.208743	10.245112	61.411463	H	54.203014	10.009200	57.694628	H	52.507165	10.087579	58.492935
H	52.177672	10.293235	59.544256	H	56.922872	9.951338	57.735595	H	55.135768	9.806235	57.869053
H	57.393855	11.152360	59.649439	H	60.540211	10.783544	61.424934	H	59.592180	10.283351	60.550400
H	59.239902	11.170840	61.648137	H	60.478824	11.036071	64.147313	H	60.231524	10.574950	63.195430
H	52.772128	12.798270	62.139123	H	52.430577	12.864684	62.165400	H	52.519725	12.817238	62.193027
H	52.528939	13.042128	64.669852	H	53.770958	12.722087	64.315407	H	53.449870	12.924710	64.549127
H	53.357697	14.597366	64.580296	H	54.446839	14.324215	63.998201	H	54.193695	14.486900	64.173152
H	53.486782	6.732247	70.660822	H	53.402687	6.289279	69.857906	H	53.673311	6.382639	70.637216
H	55.924343	2.697565	65.754804	H	56.375168	2.650692	64.934360	H	56.456184	2.360004	64.844358
H	57.675182	7.925278	63.336283	H	58.818368	7.694595	63.614264	H	59.228778	7.327322	63.577033
H	52.286031	8.162055	61.817381	H	53.707620	8.225269	61.094220	H	52.472824	7.933140	62.258592
H	51.850739	14.250003	62.584252	H	52.044114	14.221163	63.251340	H	51.946429	14.267660	63.047864
H	53.553953	14.386111	62.087233	H	53.113265	14.474726	61.850597	H	53.250161	14.396314	61.842501
O	52.818415	7.959774	64.962565	O	54.693051	7.852176	64.240665	O	54.396351	7.705210	64.876286
H	53.090237	8.937705	65.173905	H	55.253311	8.665833	64.424960	H	55.029941	8.490792	64.863698
H	51.845419	8.026536	64.918057	H	53.803900	8.228662	64.446438	H	53.628825	8.102766	65.343778
O	55.787171	8.021945	63.712181	O	58.115309	7.754324	65.219754	O	58.340355	7.378955	65.106929
H	55.829832	8.814547	63.094244	H	57.878499	8.720973	65.315816	H	58.064181	8.339812	65.117101
H	55.808752	8.522431	64.570681	H	58.799522	7.623664	65.902354	H	58.961496	7.318508	65.856421
H	51.908222	1.416894	63.964429	H	52.169790	1.198632	63.590156	H	52.005654	1.258132	63.719850

Heme (Fe³⁺) without HSO₃⁻

S=1/2			S=3/2			S=5/2					
C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000
C	50.711626	5.862154	71.439369	C	51.524650	5.332672	71.806603	C	51.128274	5.652804	71.974449
C	49.905259	6.511193	70.319061	C	51.809302	6.147026	70.547028	C	51.665304	6.336793	70.721333
N	50.367238	7.878299	70.086696	N	52.970986	7.014319	70.768828	N	52.439941	7.527484	71.081237
C	49.984836	8.639992	69.051949	C	53.412361	7.939194	69.920834	C	53.122055	8.273576	70.213600
N	49.046338	8.208444	68.196806	N	52.850300	8.070286	68.704132	N	53.093316	7.967165	68.905981
N	50.550624	9.828489	68.822217	N	54.431126	8.741684	70.254365	N	53.861708	9.303055	70.643140
C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000
C	53.640328	2.703468	63.717715	C	53.734482	2.385086	63.561698	C	53.702594	2.633235	63.472038
C	53.781738	2.931356	65.224580	C	54.078570	2.509088	65.052338	C	54.224019	2.440477	64.901316
N	55.088111	3.480983	65.597775	N	55.457951	2.924041	65.314997	N	55.563255	3.002500	65.104471
C	55.440362	4.758272	65.443285	C	55.897006	4.181832	65.181445	C	55.818451	4.314537	65.157757

N	54.529709	5.699435	65.181020	N	55.037931	5.129312	64.753307	N	54.815027	5.190630	65.272342
N	56.739446	5.112663	65.505548	N	57.164579	4.504123	65.427331	N	57.078353	4.766658	65.080878
C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000
C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000
C	57.856384	6.237284	61.325599	C	57.952776	6.189083	61.381185	C	57.786194	6.214451	61.411644
C	59.322445	6.425369	61.689052	C	59.433542	6.248735	61.741008	C	59.230915	6.422008	61.847286
N	59.614532	7.851823	62.052193	N	59.721060	7.404354	62.646639	N	59.394674	7.684995	62.640609
C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000
C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000
C	52.930334	5.832624	60.335398	C	53.180295	5.737205	60.205391	C	53.262121	5.687500	60.144227
C	53.777085	6.108478	61.570438	C	53.751815	6.147063	61.552783	C	53.801510	6.156752	61.480934
N	53.928899	7.567458	61.843727	N	54.323711	7.535114	61.549724	N	54.561352	7.443208	61.391846
Fe	55.105608	10.734416	61.715900	Fe	54.765643	10.711954	63.663680	Fe	55.531513	10.652876	62.855908
C	58.115751	11.847311	62.738023	C	57.901860	9.950693	64.778943	C	57.839176	10.422039	65.417939
C	53.880418	10.848585	64.877396	C	53.730856	11.146029	66.833996	C	52.991507	10.349518	65.151118
C	52.047047	9.983538	60.464387	C	51.553899	10.253428	62.587852	C	53.263670	10.103265	60.295009
C	56.564017	9.326801	58.907162	C	55.883513	10.704992	60.440860	C	58.078986	10.618246	60.548981
N	55.818644	11.391829	63.405281	N	55.570334	10.252042	65.425695	N	55.457411	10.325647	64.887057
C	57.048115	11.948759	63.613529	C	56.886904	9.880897	65.685886	C	56.521226	10.335176	65.770060
C	57.169409	12.572432	64.995318	C	57.077947	9.607110	67.174035	C	56.054622	10.289627	67.225429
C	58.376153	12.075048	65.816674	C	56.679437	8.138141	67.546502	C	56.392743	8.914707	67.863301
C	57.161729	14.137570	64.904205	C	58.469516	9.935150	67.729585	C	56.579642	11.465704	68.101416
C	58.392424	14.862752	64.285767	C	59.666530	8.988174	67.459924	C	58.002732	11.359701	68.730751
O	59.421545	14.199812	63.971849	O	59.594243	8.026472	66.598785	O	58.852580	10.572140	68.224914
O	58.217983	16.104792	64.172580	O	60.691920	9.235140	68.120034	O	58.163864	12.124801	69.716447
C	55.881387	12.134092	65.591324	C	55.957912	10.466111	67.696740	C	54.587208	10.432840	67.024435
C	55.139589	11.468939	64.659898	C	55.050409	10.677982	66.681389	C	54.289060	10.409178	65.676531
N	53.384358	10.387750	62.533967	N	53.018615	10.769735	64.531700	N	53.541117	10.267849	62.765151
C	53.073470	10.391939	63.885791	C	52.779185	11.079548	65.851247	C	52.673958	10.219712	63.821835
C	51.663681	9.852246	64.145641	C	51.293097	11.269514	66.134170	C	51.239926	9.976224	63.381615
C	51.743791	8.459044	64.818505	C	50.783347	10.393516	67.294563	C	50.704489	8.647188	63.963534
C	50.838740	10.818092	65.031508	C	51.028889	12.773704	66.445467	C	50.342049	11.166384	63.834042
C	49.464161	10.261284	65.442946	C	49.543155	13.146450	66.711911	C	48.845328	11.045549	63.433085
O	49.108288	10.497496	66.654626	O	49.393627	14.189244	67.405334	O	48.084177	11.755132	64.148866
O	48.790503	9.625434	64.603328	O	48.649184	12.415987	66.202558	O	48.536172	10.306579	62.462931
C	51.151524	9.770627	62.742528	C	50.719366	10.858901	64.826363	C	51.412537	9.920626	61.910947
C	52.163281	10.084626	61.872038	C	51.741026	10.600829	63.934486	C	52.746891	10.103393	61.600844
N	54.458965	9.851634	60.047494	N	53.910100	10.472093	61.904438	N	55.652414	10.332253	60.866880
C	53.111172	9.820799	59.628436	C	52.558275	10.240158	61.644567	C	54.598093	10.237764	59.966457
C	53.030365	9.384250	58.254689	C	52.350956	10.094750	60.227374	C	55.091750	10.250945	58.611765
C	54.296797	9.091387	57.854371	C	53.557543	10.322757	59.618356	C	56.447319	10.379564	58.683418
C	55.179521	9.405764	58.955456	C	54.524000	10.547076	60.654466	C	56.793979	10.440337	60.078178
N	56.957814	10.503804	61.036095	N	56.532206	10.419549	62.791974	N	57.530721	10.517555	62.955634
C	57.388422	9.870193	59.873431	C	56.833472	10.650091	61.448295	C	58.424395	10.669491	61.893953
C	58.816696	10.015440	59.727375	C	58.252161	10.690599	61.263008	C	59.753398	10.843243	62.392335
C	59.241789	10.808629	60.760736	C	58.823815	10.463210	62.495595	C	59.678834	10.776292	63.766364
C	58.086388	11.103064	61.568335	C	57.746551	10.288968	63.425044	C	58.304929	10.575031	64.099894
C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000
C	54.253354	13.891437	62.088345	C	53.750586	13.801691	63.857855	C	53.939427	13.514163	63.664173
S	54.712872	12.655206	60.829882	S	55.243992	12.775473	63.709023	S	55.495080	12.933944	62.885483
H	54.827799	6.666370	64.980318	H	55.237023	6.125583	64.854733	H	54.939724	6.180517	65.019506
H	50.908215	3.944548	72.445235	H	50.149603	3.827594	72.549090	H	49.944677	3.921984	72.539397
H	50.527847	3.816196	70.716160	H	50.507418	3.674906	70.818337	H	50.957996	3.658116	71.107597
H	49.264567	4.287555	71.871315	H	49.416730	4.955410	71.393102	H	49.474416	4.631886	70.983019
H	50.546477	6.420743	72.372930	H	51.339206	6.024852	72.641301	H	50.492024	6.362604	72.524151
H	51.782501	5.944166	71.198775	H	52.422877	4.750628	72.062906	H	51.972819	5.396749	72.631467
H	50.024360	5.931798	69.389876	H	52.009598	5.476933	69.696481	H	52.315526	5.644832	70.164081
H	48.835586	6.512643	70.580467	H	50.936574	6.769481	70.298413	H	50.827527	6.626653	70.067033

H	48.734078	8.896302	67.488613	H	53.013140	8.928453	68.181940	H	53.545736	8.577834	68.230646
H	48.437602	7.443426	68.456656	H	51.955288	7.624778	68.534319	H	52.373223	7.348447	68.554022
H	50.179503	10.372138	68.012680	H	54.871767	9.311977	69.537227	H	54.331331	9.922568	69.996869
H	51.292795	10.175159	69.414297	H	54.954849	8.580977	71.105938	H	53.985731	9.483141	71.631097
H	52.149365	2.056798	62.273714	H	51.991180	2.107834	62.287911	H	51.882977	2.366643	62.310409
H	51.491148	3.047825	63.591394	H	51.705108	3.178788	63.673807	H	51.600792	2.919707	63.972517
H	53.902377	3.631182	63.188391	H	54.123040	3.260318	63.020595	H	53.847629	3.682947	63.177523
H	54.372630	1.946756	63.403588	H	54.255632	1.511618	63.147933	H	54.313869	2.028772	62.787956
H	53.668963	1.990004	65.772608	H	53.934295	1.550314	65.559904	H	54.289330	1.376434	65.149917
H	52.988682	3.593840	65.598843	H	53.396334	3.215898	65.550652	H	53.531017	2.877946	65.636039
H	53.545882	5.501741	65.311506	H	54.050469	4.902603	64.754921	H	53.865202	4.848639	65.340657
H	57.435417	4.411798	65.731697	H	57.820244	3.788019	65.715043	H	57.843777	4.107705	65.015485
H	56.971401	6.068282	65.750085	H	57.523773	5.462152	65.240948	H	57.313419	5.742015	65.287063
H	57.364380	2.730542	61.228438	H	57.310048	2.736565	61.247629	H	57.503031	2.713222	61.208122
H	56.904926	3.827384	62.549201	H	56.946489	3.856837	62.576612	H	56.809722	3.756670	62.464160
H	58.619007	3.543564	62.179157	H	58.629642	3.506046	62.139391	H	58.574323	3.626703	62.280181
H	58.298110	4.664705	59.912892	H	58.257414	4.649055	59.883680	H	58.347189	4.712982	59.950437
H	56.592416	4.870725	60.253921	H	56.574244	4.924968	60.301020	H	56.615473	4.847641	60.210131
H	57.230055	6.400669	62.218006	H	57.354817	6.319693	62.298599	H	57.129114	6.285472	62.295421
H	57.573433	7.004366	60.587980	H	57.714574	7.026331	60.707538	H	57.520420	7.030123	60.718814
H	59.969420	6.174836	60.841945	H	60.056322	6.347282	60.846431	H	59.891737	6.492414	60.978110
H	59.620261	5.812593	62.545427	H	59.748391	5.352774	62.285225	H	59.585553	5.606946	62.485394
H	59.421623	8.502532	61.263181	H	59.443203	8.310450	62.229650	H	58.992926	8.508500	62.157265
H	60.600444	7.975182	62.304417	H	60.717543	7.460762	62.876653	H	60.386763	7.900277	62.787332
H	51.576813	2.800502	59.139561	H	51.402943	2.867561	59.205854	H	51.335361	2.903078	59.223999
H	52.492161	3.977359	58.173933	H	52.547593	3.793267	58.213442	H	52.562192	3.721028	58.235262
H	50.913335	4.423032	58.856019	H	51.029391	4.542762	58.750958	H	51.082843	4.583161	58.709394
H	53.433589	3.744171	60.494662	H	53.300783	3.626490	60.625495	H	53.251127	3.597575	60.670821
H	51.874925	4.172811	61.189782	H	51.797442	4.383315	61.145964	H	51.783019	4.466364	61.125662
H	52.029691	6.465953	60.352832	H	52.431765	6.478867	59.886803	H	52.573890	6.446106	59.742167
H	53.494401	6.098485	59.428874	H	53.972850	5.725741	59.441980	H	54.083304	5.576217	59.419709
H	54.783768	5.687014	61.471629	H	54.553053	5.475365	61.883883	H	54.483617	5.421037	61.925399
H	53.313320	5.675061	62.464518	H	52.969005	6.148052	62.319785	H	52.984857	6.331584	62.191348
H	54.331765	8.106701	61.048550	H	55.178104	7.607149	60.986352	H	55.437231	7.342718	60.867922
H	54.522990	7.776867	62.689544	H	54.531160	7.839487	62.531038	H	54.776297	7.763375	62.368193
H	59.031242	12.362455	63.027881	H	58.911803	9.751300	65.125931	H	58.551964	10.484058	66.246083
H	53.507306	10.848403	65.899248	H	53.430011	11.472517	67.828365	H	52.173695	10.361498	65.867877
H	51.044246	9.885526	60.053284	H	50.532044	10.094356	62.250089	H	52.546220	10.015509	59.482065
H	57.024467	8.915080	58.011974	H	56.228693	10.814436	59.414317	H	58.876845	10.729437	59.817112
H	59.311424	12.338907	65.314666	H	57.415543	7.418921	67.181789	H	57.480040	8.798321	67.913685
H	58.318166	10.990234	65.981672	H	55.688459	7.891158	67.144633	H	55.945016	8.095354	67.285130
H	58.364657	12.558726	66.801432	H	56.642193	8.050344	68.639323	H	56.011575	8.865362	68.892081
H	56.275826	14.460902	64.342545	H	58.775305	10.934350	67.388601	H	56.545811	12.394230	67.513764
H	57.030825	14.523693	65.925688	H	58.393841	10.004594	68.823251	H	55.876457	11.610485	68.933445
H	55.574674	12.341882	66.612038	H	55.841448	10.788306	68.728394	H	53.848975	10.603584	67.804658
H	52.371746	7.774024	64.232513	H	50.948084	9.330784	67.075646	H	51.358537	7.806418	63.689459
H	50.743342	8.020675	64.898384	H	49.708964	10.560020	67.419296	H	49.704374	8.460230	63.559559
H	52.179766	8.552341	65.822965	H	51.286676	10.659324	68.232914	H	50.644793	8.706784	65.057675
H	50.680408	11.761215	64.489039	H	51.358011	13.386393	65.593799	H	50.721564	12.099063	63.396169
H	51.412296	11.061860	65.933892	H	51.636028	13.071418	67.310452	H	50.406914	11.274652	64.924036
H	50.134790	9.500392	62.482014	H	49.656697	10.828484	64.616678	H	50.599417	9.778469	61.208919
H	52.103502	9.276125	57.700526	H	51.389299	9.895460	59.764408	H	54.461517	10.181203	57.731131
H	54.629549	8.709515	56.894139	H	53.782742	10.328376	58.556637	H	57.164377	10.442689	57.871023
H	59.391936	9.625607	58.892855	H	58.746145	10.870478	60.313604	H	60.628552	10.998702	61.769086
H	60.241590	11.181340	60.963066	H	59.876809	10.470984	62.763553	H	60.479958	10.865787	64.492835
H	52.728108	12.853620	63.236978	H	52.414712	12.767677	62.490882	H	52.583218	12.847629	62.098569
H	55.002801	13.881252	62.886851	H	53.227724	13.516864	64.778081	H	53.626915	12.777646	64.412841
H	54.378274	14.840522	61.545991	H	54.161896	14.809724	64.015751	H	54.201050	14.437919	64.195612

H	51.067649	8.253872	70.716132	H	53.473613	6.902122	71.644058	H	52.451278	7.806042	72.057087
H	55.820411	2.823314	65.844436	H	56.135495	2.212129	65.563744	H	56.352641	2.365946	65.113266
H	59.032446	8.185390	62.858190	H	59.163853	7.285747	63.555207	H	58.953270	7.611198	63.596970
H	53.006050	8.003275	62.010004	H	53.647756	8.212393	61.156175	H	54.012604	8.190206	60.915987
H	52.614837	14.625956	63.287734	H	52.005755	14.470148	62.781301	H	51.932912	14.133653	63.146224
H	52.098462	13.739728	61.830859	H	53.381923	14.048590	61.731877	H	53.147995	14.517645	61.904897
O	55.334486	8.209214	64.185646	O	54.475497	7.909298	64.358007	O	54.735591	7.744569	64.159960
H	56.286422	8.502432	64.141836	H	54.876590	8.695085	64.838009	H	55.201266	8.596876	64.406032
H	54.834578	8.994676	64.529046	H	53.532572	7.953867	64.604524	H	53.805762	7.972971	64.366651
O	57.967606	8.976710	64.054567	O	58.155381	7.046007	64.834144	O	58.306381	7.459588	65.216964
H	57.968874	9.917439	63.746347	H	57.499248	7.750492	64.662518	H	57.997609	8.383349	65.415039
H	58.391320	9.012871	64.932380	H	58.718663	7.493588	65.639941	H	59.042729	7.324977	65.842487
H	51.938146	1.355294	63.885701	H	51.808665	1.423611	63.911067	H	52.045593	1.230430	63.658065

Heme (Fe²⁺) without SO₃²⁻

S=0			S=1			S=2					
C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000
C	50.234814	5.595128	70.688677	C	50.248341	5.597030	70.688561	C	50.318436	5.617960	70.714890
C	51.613937	6.082097	70.256295	C	51.626522	6.165638	70.355130	C	51.731821	6.051521	70.341550
N	51.488438	7.247871	69.379221	N	51.486386	7.304403	69.442918	N	51.687433	7.237246	69.483265
C	52.471614	7.751416	68.637490	C	52.438199	7.788750	68.650192	C	52.701194	7.691134	68.758555
N	53.710627	7.271397	68.707561	N	53.697513	7.361472	68.731294	N	53.907583	7.133699	68.818339
N	52.209084	8.736736	67.732867	N	52.116784	8.685730	67.672220	N	52.509124	8.718131	67.868129
C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000
C	53.730366	2.522245	63.415279	C	53.741572	2.459388	63.375598	C	53.715652	2.594203	63.414211
C	54.275776	2.415665	64.855254	C	54.282651	2.457705	64.821221	C	54.251830	2.496664	64.854243
N	55.348681	3.370297	65.137593	N	55.388023	3.392480	65.051787	N	55.376689	3.398785	65.112777
C	55.131328	4.678224	65.297030	C	55.211478	4.712096	65.122719	C	55.238095	4.712448	65.273941
N	53.897089	5.167346	65.349376	N	54.018021	5.238544	64.853696	N	54.023529	5.264786	65.335955
N	56.182765	5.545801	65.355865	N	56.260817	5.534236	65.413789	N	56.320351	5.532020	65.317532
C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000
C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000
C	56.825988	6.052271	61.313337	C	57.240267	6.167450	61.444960	C	56.799400	6.046670	61.292330
C	57.672721	6.818771	62.323559	C	58.362458	6.648966	62.367601	C	57.639187	6.872067	62.261665
N	56.806784	7.609470	63.258679	N	57.820598	7.358388	63.570907	N	56.770603	7.653110	63.201743
C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000
C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000
C	51.710893	5.407910	61.081193	C	53.143977	5.747296	60.153873	C	51.860304	5.597662	60.923628
C	52.536258	6.080879	62.167154	C	53.451596	6.390157	61.494462	C	52.454966	5.944845	62.278348
N	51.731229	6.969098	63.061630	N	54.112206	7.717370	61.306684	N	51.830963	7.169809	62.870698
Fe	55.144610	10.656360	63.877024	Fe	55.238892	10.572286	63.028487	Fe	55.099962	10.710816	64.042071
C	57.209351	10.825943	66.537635	C	56.995044	10.660733	65.951055	C	57.352438	10.526287	66.649086
C	52.374180	11.334763	65.824720	C	52.307359	10.640338	64.756243	C	52.567533	11.360496	66.223705
C	52.962444	9.611841	61.330415	C	53.505456	10.419558	60.066706	C	52.838031	9.751861	61.621803
C	57.762601	10.261579	61.762123	C	58.182328	10.005988	61.273316	C	57.654059	10.325501	61.789898
N	54.891498	10.975115	65.766553	N	54.776911	10.731324	64.938339	N	55.007741	10.875142	66.074672
C	55.863142	11.051508	66.737949	C	55.652875	10.939373	65.984432	C	56.039968	10.838779	66.959042
C	55.312013	11.472254	68.093743	C	54.953044	11.477360	67.231406	C	55.606723	11.244849	68.364178
C	55.578483	10.459017	69.224957	C	55.321442	10.760265	68.540361	C	55.902173	10.184653	69.442855
C	55.810540	12.903371	68.488108	C	55.224222	13.013132	67.343924	C	56.227826	12.628853	68.756867
C	57.269054	13.114094	68.994324	C	56.682509	13.503914	67.561579	C	57.724429	12.729712	69.176184
O	58.057238	12.130285	69.100335	O	57.514319	12.739759	68.135942	O	58.457869	11.699436	69.190914
O	57.520650	14.318055	69.271260	O	56.898636	14.679594	67.156047	O	58.065353	13.904040	69.485716
C	53.867149	11.577139	67.757124	C	53.524992	11.271623	66.823828	C	54.144390	11.447557	68.135782
C	53.668252	11.313991	66.436345	C	53.483975	10.911021	65.499902	C	53.859580	11.279481	66.804701
N	53.052096	10.245523	63.748965	N	53.342662	10.309033	62.560940	N	53.135565	10.504817	63.995156
C	52.061042	10.831817	64.630264	C	52.255683	10.348867	63.431669	C	52.238878	10.945854	64.977705
C	50.657743	10.692282	64.061912	C	50.929375	10.095755	62.709353	C	50.784604	10.824479	64.521306
C	49.889671	9.602340	64.856870	C	50.412198	8.671422	63.035023	C	50.041213	9.779289	65.388156

C	49.859875	12.011167	64.100518	C	49.845175	11.131355	63.084215	C	50.044266	12.179602	64.592090
C	48.424177	11.955615	63.513465	C	48.464213	10.945055	62.402752	C	48.574479	12.185414	64.092100
O	47.683191	12.922498	63.845002	O	47.496697	11.473475	63.021683	O	47.919759	13.217711	64.409279
O	48.122063	10.989669	62.752644	O	48.414377	10.318341	61.305678	O	48.160558	11.201413	63.411860
C	50.975218	10.234090	62.670549	C	51.386742	10.205915	61.294790	C	50.981613	10.343025	63.123670
C	52.304941	10.012981	62.510435	C	52.750193	10.340151	61.252187	C	52.317336	10.194921	62.859252
N	55.331212	9.932729	62.044583	N	55.733186	10.211677	61.102366	N	55.237915	9.969375	62.154818
C	54.314490	9.587249	61.121584	C	54.880240	10.335587	60.003847	C	54.178834	9.699844	61.287895
C	54.894519	9.325125	59.824225	C	55.630079	10.252416	58.775179	C	54.672822	9.517738	59.948844
C	56.226112	9.584875	59.914359	C	56.939159	10.073158	59.115338	C	56.019307	9.766620	59.977075
C	56.501215	9.969578	61.275985	C	57.008683	10.071454	60.552730	C	56.371828	10.060498	61.334735
N	57.082049	10.490821	64.109754	N	57.155318	10.232665	63.516846	N	57.078746	10.445931	64.189876
C	58.050702	10.446941	63.107092	C	58.263115	10.092105	62.657179	C	57.997201	10.452371	63.128658
C	59.364368	10.492774	63.685912	C	59.465420	10.010677	63.414755	C	59.332902	10.436872	63.644184
C	59.202759	10.558597	65.044764	C	59.117347	10.128470	64.746851	C	59.240220	10.390160	65.013134
C	57.789196	10.597673	65.298750	C	57.703171	10.310362	64.795978	C	57.845179	10.428841	65.346437
C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000
C	53.894391	13.710983	63.734607	C	54.092903	13.609903	63.489834	C	53.746713	13.830060	63.861367
S	55.369864	12.724348	63.306520	S	55.424727	12.684711	62.651268	S	55.344556	12.961896	63.638361
H	53.684084	6.210296	65.300145	H	53.793060	6.242363	64.944558	H	53.891974	6.282743	65.358181
H	49.331836	4.054518	71.924784	H	49.328430	4.011266	71.851125	H	49.308878	4.098338	71.892021
H	50.883580	4.650645	72.542932	H	50.806644	4.666494	72.581120	H	50.871549	4.602405	72.562260
H	50.844894	3.552059	71.146684	H	50.912982	3.578414	71.180072	H	50.814906	3.537732	71.140440
H	49.651265	5.333044	69.794093	H	49.747653	5.310876	69.751692	H	49.755623	5.401842	69.795171
H	49.706309	6.420711	71.189088	H	49.640409	6.390509	71.149542	H	49.809798	6.454932	71.216687
H	52.217351	6.344143	71.139519	H	52.144454	6.482676	71.273339	H	52.315479	6.273372	71.248438
H	52.141413	5.289078	69.705987	H	52.243635	5.401044	69.860411	H	52.245049	5.247673	69.793342
H	54.418885	7.550579	68.007227	H	54.395108	7.644819	68.029363	H	54.645888	7.422822	68.160787
H	53.974022	6.633649	69.448371	H	54.000775	6.801661	69.518356	H	54.142988	6.487805	69.562283
H	52.904520	9.493739	67.660962	H	52.776273	9.484953	67.499754	H	53.192449	9.503332	67.944687
H	51.255429	9.088886	67.718629	H	51.146996	8.995487	67.673343	H	51.560042	9.090027	67.848871
H	51.863396	2.253325	62.312262	H	51.853470	2.206498	62.317340	H	51.863850	2.217660	62.313752
H	51.664604	3.042687	63.889699	H	51.704491	3.101709	63.840400	H	51.625447	3.019098	63.880969
H	53.958121	3.525636	63.028294	H	54.005227	3.408788	62.888006	H	53.898223	3.610029	63.036685
H	54.272073	1.820993	62.767525	H	54.243462	1.674978	62.795874	H	54.291659	1.922114	62.765359
H	54.676503	1.418032	65.056174	H	54.645311	1.466373	65.105096	H	54.597708	1.484368	65.081637
H	53.469178	2.567954	65.588838	H	53.476353	2.706716	65.529047	H	53.455087	2.710479	65.582735
H	53.117849	4.520919	65.371194	H	53.231135	4.622867	64.685590	H	53.204411	4.679105	65.437252
H	57.097957	5.122307	65.488091	H	57.038393	5.074832	65.883698	H	57.226960	5.075628	65.379418
H	56.027753	6.403062	65.929706	H	55.998355	6.447056	65.859928	H	56.221469	6.376151	65.924662
H	58.167496	2.811356	61.316582	H	57.847178	2.725389	61.219347	H	58.195038	2.823374	61.329403
H	56.603717	3.338976	61.974171	H	56.651089	3.555249	62.233013	H	56.605157	3.318250	61.950146
H	58.123818	3.948953	62.670410	H	58.390404	3.809015	62.505729	H	58.096476	3.960597	62.681472
H	58.603696	5.148024	60.447386	H	58.548683	4.947458	60.212775	H	58.604041	5.161892	60.464628
H	57.084578	4.525146	59.807129	H	56.828781	4.654446	59.956853	H	57.107065	4.515441	59.798616
H	55.912472	5.679607	61.808670	H	56.334788	5.991577	62.051831	H	55.907674	5.659690	61.816664
H	56.498301	6.742532	60.523981	H	57.017405	6.960518	60.714341	H	56.433327	6.701087	60.489525
H	58.344901	7.528018	61.832537	H	59.031901	7.347428	61.858582	H	58.271506	7.593321	61.735783
H	58.271522	6.150822	62.951823	H	58.956440	5.813185	62.748948	H	58.279595	6.242509	62.888865
H	56.103835	8.195718	62.753815	H	57.257125	8.203234	63.328497	H	56.039319	8.226948	62.716044
H	57.344756	8.298085	63.810429	H	58.584121	7.745817	64.149879	H	57.298442	8.365605	63.737468
H	52.429025	3.078386	58.558763	H	51.424850	2.855409	59.188310	H	52.330249	2.961828	58.660309
H	51.704182	4.684838	58.334150	H	52.541544	3.824606	58.206290	H	51.864052	4.628265	58.262323
H	50.845566	3.446116	59.272600	H	51.014122	4.532493	58.772136	H	50.785566	3.615612	59.245236
H	53.509030	4.786319	60.057754	H	53.313864	3.645614	60.631139	H	53.587940	4.579542	60.114546
H	52.743582	3.507927	60.989118	H	51.795015	4.386466	61.143919	H	52.527970	3.549074	61.069136
H	50.824441	4.933816	61.531058	H	52.439487	6.400574	59.616581	H	50.781237	5.414808	61.043758
H	51.341793	6.170596	60.379688	H	54.057019	5.688755	59.542164	H	51.969730	6.451663	60.238397

H	53.324515	6.709440	61.733982	H	54.117525	5.777078	62.113765	H	53.530797	6.152379	62.203368
H	53.011766	5.338520	62.819676	H	52.531986	6.568777	62.062052	H	52.306774	5.129160	62.992864
H	51.406166	7.819857	62.574455	H	55.117030	7.640699	61.109052	H	52.074902	8.021152	62.307628
H	52.347720	7.308893	63.918199	H	54.002436	8.378636	62.109701	H	52.191884	7.368604	63.829581
H	57.852218	10.958180	67.409475	H	57.565377	10.863314	66.855706	H	58.065276	10.581547	67.472625
H	51.569719	11.738763	66.439205	H	51.363705	10.711067	65.293865	H	51.764660	11.699692	66.876665
H	52.327078	9.393662	60.472562	H	52.952790	10.499522	59.132561	H	52.118698	9.619580	60.812752
H	58.590830	10.263761	61.055668	H	59.115035	9.914489	60.718324	H	58.455975	10.363538	61.054601
H	56.652364	10.406820	69.426263	H	56.365381	10.966273	68.798201	H	56.983097	10.050132	69.547181
H	55.197473	9.464844	68.962875	H	55.161483	9.678216	68.460739	H	55.425373	9.228201	69.198960
H	55.068494	10.791414	70.138550	H	54.686679	11.141070	69.352128	H	55.500459	10.527938	70.405496
H	55.664080	13.575056	67.631381	H	54.843681	13.504449	66.440210	H	56.073836	13.331484	67.926426
H	55.148765	13.274384	69.284458	H	54.622055	13.394150	68.184387	H	55.640985	13.021354	69.600007
H	53.095728	11.898479	68.452527	H	52.669661	11.640035	67.386680	H	53.444643	11.798302	68.889617
H	50.484069	8.683562	64.953735	H	51.179447	7.912966	62.827562	H	50.575151	8.818558	65.399198
H	48.948217	9.379548	64.343748	H	49.530319	8.462174	62.420541	H	49.035821	9.628147	64.980744
H	49.663587	9.973799	65.866266	H	50.137014	8.603082	64.096739	H	49.949404	10.144291	66.421694
H	50.408928	12.785605	63.549291	H	50.203294	12.140483	62.835257	H	50.593218	12.921665	63.997439
H	49.788541	12.361060	65.139851	H	49.682859	11.116536	64.169886	H	50.053623	12.544974	65.628853
H	50.213584	10.145876	61.902019	H	50.713518	10.174246	60.445388	H	50.165084	10.192763	62.425648
H	54.323938	9.016625	58.953789	H	55.189544	10.312579	57.784724	H	54.049951	9.284787	59.090727
H	56.978091	9.533304	59.132799	H	57.800002	9.973127	58.460926	H	56.721349	9.760511	59.148753
H	60.288166	10.465394	63.116211	H	60.457072	9.897063	62.986481	H	60.228176	10.439202	63.029917
H	59.964745	10.612554	65.815659	H	59.771242	10.164342	65.612697	H	60.042806	10.370030	65.743463
H	52.458635	12.762966	62.405957	H	52.404173	12.790762	62.396719	H	52.555712	12.731875	62.411538
H	53.480146	13.321946	64.673159	H	53.869692	13.126048	64.446706	H	53.248724	13.405365	64.741589
H	54.287792	14.714469	63.951371	H	54.541204	14.587704	63.718346	H	54.004633	14.870579	64.098266
H	50.611438	7.759963	69.406059	H	50.580108	7.762854	69.415050	H	50.839915	7.797595	69.504841
H	56.305522	3.035285	65.166282	H	56.304719	3.020334	65.274535	H	56.314619	3.012451	65.138716
H	56.337833	6.962367	63.920500	H	57.246738	6.712538	64.149360	H	56.342153	7.001056	63.880918
H	50.898375	6.484614	63.411895	H	53.705740	8.251864	60.513296	H	50.808134	7.099886	62.911021
H	51.987851	14.389913	62.953946	H	52.082189	14.351534	63.184734	H	51.917998	14.342559	62.819269
H	53.252032	14.189900	61.717973	H	53.059893	14.281410	61.698426	H	53.335618	14.184829	61.756968
O	53.291769	7.768327	65.026903	O	53.067646	7.817038	65.152318	O	53.321087	8.034411	65.217191
H	53.266717	9.292502	64.169216	H	52.815834	8.641214	64.657794	H	53.380350	8.934733	64.742782
H	52.700744	8.028120	65.766242	H	52.556043	7.927589	65.996374	H	52.872819	8.251022	66.082633
O	55.411840	7.944319	66.528809	O	55.421387	7.958430	66.439540	O	55.714180	7.867378	66.672251
H	54.633990	8.054600	65.878972	H	54.636720	8.143645	65.852846	H	55.002653	8.239625	66.097192
H	55.890677	8.799890	66.571774	H	55.974443	8.779074	66.397173	H	56.351468	8.617374	66.800061
H	51.967365	1.299718	63.795494	H	51.932919	1.344826	63.863185	H	52.015529	1.293998	63.808506

Heme (Fe³⁺) without SO₃²⁻

S=1/2			S=3/2			S=5/2					
C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000	C	50.331000	4.395000	71.629000
C	50.229381	5.480101	70.556138	C	50.217905	5.435125	70.515931	C	50.377646	5.923947	71.577861
C	51.600703	5.992336	70.120590	C	51.588720	5.953727	70.098080	C	51.707701	6.471507	72.112809
N	51.447148	7.053763	69.119429	N	51.454752	7.004660	69.083153	N	51.805441	7.924247	72.096124
C	52.433187	7.579771	68.395975	C	52.463004	7.525248	68.399847	C	51.453417	8.720702	73.104834
N	53.698343	7.194871	68.593829	N	53.717313	7.141570	68.620771	N	50.873807	8.211387	74.216581
N	52.158994	8.456399	67.400380	N	52.227908	8.440062	67.400665	N	51.721321	10.026446	73.024227
C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000	C	52.225000	2.268000	63.346000
C	53.663825	2.765401	63.482789	C	53.711694	2.624275	63.405682	C	53.702968	2.633259	63.446589
C	54.173821	2.632214	64.924066	C	54.262769	2.498599	64.835223	C	54.274811	2.367169	64.845489
N	55.385901	3.419848	65.188237	N	55.476561	3.289647	65.077821	N	55.574019	3.015567	65.052469
C	55.379622	4.738472	65.351104	C	55.456660	4.603077	65.281003	C	55.715146	4.344721	65.127071
N	54.240773	5.424816	65.350064	N	54.310505	5.276928	65.260564	N	54.652541	5.121718	65.353728
N	56.552988	5.436956	65.488546	N	56.614254	5.309509	65.470305	N	56.917460	4.913844	64.967152
C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000	C	57.624000	3.668000	61.733000
C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000	C	57.584000	4.849000	60.729000

C	57.274311	6.172269	61.453558	C	57.195837	6.156760	61.434110	C	57.837260	6.208206	61.408566
C	58.434106	6.641351	62.333329	C	58.329591	6.676982	62.318085	C	59.292850	6.357737	61.837968
N	57.935072	7.327121	63.574540	N	57.796207	7.335614	63.554474	N	59.496698	7.559986	62.709201
C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000	C	51.838000	3.862000	59.049000
C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000	C	52.531000	4.355000	60.326000
C	52.966076	5.819170	60.275219	C	52.563314	5.870700	60.539031	C	53.274950	5.681076	60.134741
C	53.486339	6.218702	61.641169	C	53.080971	6.140634	61.943425	C	53.892538	6.113550	61.449662
N	53.906974	7.652227	61.711301	N	53.156778	7.594990	62.280696	N	54.576278	7.446346	61.383723
Fe	55.237434	10.650341	63.070670	Fe	55.014178	10.588445	63.312995	Fe	55.381660	10.658697	63.440700
C	56.987275	10.628106	66.014554	C	56.987643	10.375780	66.130583	C	58.631158	10.460966	62.336795
C	52.293524	10.640736	64.814187	C	52.240783	10.929988	65.302093	C	56.495376	10.619877	66.698515
C	53.526908	10.527413	60.122479	C	53.004829	10.252546	60.551925	C	52.184484	9.971792	64.583246
C	58.186827	10.163923	61.346317	C	57.783497	10.109004	61.333450	C	54.261847	10.371889	60.209831
N	54.767543	10.728139	65.010721	N	54.692144	10.596227	65.326231	N	57.209342	10.539557	64.317393
C	55.635092	10.901187	66.059872	C	55.663489	10.678418	66.308096	C	58.422953	10.667576	63.676833
C	54.941979	11.431358	67.301868	C	55.115381	11.252189	67.606327	C	59.528604	11.082918	64.639748
C	55.261926	10.704045	68.617369	C	55.449525	10.484360	68.893195	C	60.695699	10.076156	64.734252
C	55.250881	12.969193	67.432106	C	55.568789	12.761088	67.711778	C	60.042476	12.530510	64.318877
C	56.668852	13.418117	67.894029	C	57.058073	13.076846	68.074447	C	61.001737	12.729972	63.101926
O	57.567929	12.554797	68.106895	O	57.864452	12.143926	68.329052	O	61.308360	11.756259	62.361385
O	56.765069	14.667264	68.008308	O	57.277115	14.315502	68.073185	O	61.384288	13.924677	63.000647
C	53.517661	11.295115	66.881672	C	53.667320	11.304936	67.285399	C	58.768000	11.149640	65.909776
C	53.457510	10.927682	65.567041	C	53.480648	10.993769	65.953070	C	57.444149	10.832768	65.686179
N	53.357429	10.459449	62.614363	N	53.058601	10.507916	63.037379	N	54.559745	10.195219	65.279140
C	52.270352	10.393494	63.481337	C	52.064403	10.619690	63.985712	C	55.199994	10.231547	66.492234
C	50.977207	10.041612	62.744830	C	50.674084	10.383974	63.415424	C	54.296042	9.740556	67.615796
C	50.531292	8.604588	63.111805	C	50.051534	9.113359	64.043831	C	54.801354	8.314057	67.996351
C	49.830024	11.040507	63.053018	C	49.747364	11.605058	63.661962	C	54.276789	10.657496	68.855301
C	48.476795	10.688447	62.383049	C	48.310115	11.478457	63.084558	C	53.369988	10.193683	70.009923
O	47.458440	11.021892	63.049061	O	47.490715	12.298417	63.582214	O	53.478493	10.855427	71.083869
O	48.506273	10.129241	61.250650	O	48.092980	10.616206	62.189167	O	52.587392	9.212004	69.825088
C	51.436564	10.148977	61.336194	C	51.003098	10.219082	61.977867	C	52.990592	9.679404	66.903837
C	52.784626	10.404176	61.314567	C	52.364339	10.339563	61.798703	C	53.187749	9.952141	65.563699
N	55.740980	10.352042	61.174281	N	55.314466	10.135212	61.399470	N	53.617829	10.303264	62.592380
C	54.886577	10.484115	60.058402	C	54.362761	10.159778	60.375279	C	52.388126	10.164029	63.228739
C	55.648127	10.463705	58.833473	C	55.003437	10.051695	59.089403	C	51.325809	10.179233	62.256869
C	56.951478	10.309118	59.181568	C	56.345795	10.000699	59.312970	C	51.903150	10.314764	61.025054
C	57.003755	10.257650	60.624483	C	56.544962	10.070536	60.734000	C	53.321892	10.375907	61.227606
N	57.142651	10.272306	63.575159	N	56.952855	10.213121	63.651996	N	56.256692	10.320738	61.661741
C	58.253921	10.178572	62.720259	C	57.987074	10.170928	62.704383	C	55.631655	10.282546	60.410470
C	59.468610	10.097071	63.484989	C	59.254948	10.093130	63.353734	C	56.609062	10.146727	59.375173
C	59.116259	10.172938	64.803935	C	59.012677	10.078188	64.710170	C	57.838883	10.129819	59.986888
C	57.686287	10.326374	64.853418	C	57.598879	10.188245	64.885109	C	57.608234	10.270753	61.395247
C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000	C	52.837000	13.766000	62.641000
C	54.028733	13.637571	63.581811	C	53.891141	13.597200	63.722757	C	53.610035	13.416925	63.908367
S	55.460518	12.779533	62.849896	S	55.370272	12.670661	63.206765	S	55.345125	12.929930	63.559917
H	54.243321	6.450352	65.248417	H	54.280695	6.309955	65.282613	H	54.668703	6.116558	65.090832
H	49.332395	4.047214	71.917880	H	49.339873	4.020590	71.909255	H	49.375177	4.017846	71.244868
H	50.830459	4.773234	72.530816	H	50.794924	4.825110	72.525895	H	50.445698	4.029835	72.659095
H	50.898044	3.527044	71.265526	H	50.937082	3.535905	71.311917	H	51.135956	3.952131	71.025337
H	49.698075	5.093199	69.674176	H	49.713081	5.005220	69.639074	H	50.243262	6.276888	70.544440
H	49.641653	6.327841	70.940068	H	49.605748	6.282322	70.859048	H	49.543427	6.346015	72.159272
H	52.152150	6.381901	70.990790	H	52.123145	6.360274	70.970906	H	51.888984	6.108027	73.135209
H	52.191097	5.176464	69.678102	H	52.193680	5.137858	69.675521	H	52.534607	6.088489	71.499969
H	54.461605	7.527268	67.999965	H	54.498760	7.430710	68.020251	H	50.571946	8.846195	74.945072
H	53.946919	6.686361	69.433728	H	53.938190	6.571719	69.428756	H	50.381119	7.328947	74.161561
H	52.813108	9.239907	67.252083	H	52.810424	9.295119	67.457893	H	51.394101	10.650047	73.750370
H	51.185524	8.728358	67.296673	H	51.246784	8.688179	67.283515	H	52.373259	10.383365	72.277317

H	51.901300	2.287514	62.300362	H	51.868804	2.219831	62.312213	H	51.850855	2.414653	62.327155
H	51.532978	2.890152	63.929404	H	51.615327	3.005837	63.885663	H	51.619004	2.885736	64.022802
H	53.718032	3.819489	63.175693	H	53.863961	3.650805	63.045711	H	53.829808	3.699728	63.211110
H	54.335191	2.211338	62.813347	H	54.293850	1.977243	62.738068	H	54.296378	2.074980	62.709242
H	54.418327	1.591507	65.155883	H	54.513578	1.459202	65.064691	H	54.424364	1.295956	65.012648
H	53.397514	2.931379	65.644666	H	53.502538	2.797081	65.573540	H	53.575000	2.697045	65.627828
H	53.355933	4.941419	65.258961	H	53.433776	4.779916	65.166122	H	53.749942	4.696097	65.520213
H	57.360354	4.860229	65.719034	H	57.432130	4.741612	65.683422	H	57.727000	4.341736	64.765630
H	56.477399	6.269156	66.108497	H	56.514703	6.121092	66.114638	H	57.056673	5.917501	65.109199
H	57.834988	2.723500	61.218343	H	57.899642	2.732723	61.231731	H	57.497115	2.713191	61.209734
H	56.654351	3.562990	62.241280	H	56.635644	3.524524	62.193203	H	56.811193	3.757734	62.464870
H	58.399106	3.802233	62.498709	H	58.354004	3.835250	62.536411	H	58.576733	3.619713	62.275021
H	58.539756	4.933130	60.194144	H	58.558932	4.966964	60.236161	H	58.325592	4.694975	59.933137
H	56.811223	4.667213	59.971724	H	56.853525	4.634980	59.938592	H	56.604301	4.869994	60.232018
H	56.393443	6.002736	62.097579	H	56.310619	5.956442	62.064379	H	57.189277	6.297755	62.297350
H	57.015014	6.965142	60.737186	H	56.903382	6.933533	60.714931	H	57.592139	7.035637	60.723082
H	59.084235	7.350592	61.813807	H	58.945418	7.417974	61.800889	H	59.949780	6.466511	60.970003
H	59.044820	5.803313	62.681093	H	58.980881	5.868863	62.664242	H	59.632589	5.495524	62.419639
H	57.360962	8.166864	63.360562	H	57.136995	8.105171	63.332718	H	59.210980	8.454555	62.255995
H	58.718743	7.689636	64.137866	H	58.548897	7.801033	64.090169	H	60.482592	7.667528	62.971468
H	51.549263	2.808858	59.147630	H	51.854991	2.766069	59.005233	H	51.318506	2.913305	59.229100
H	52.500465	3.951059	58.177796	H	52.336583	4.244339	58.148052	H	52.565678	3.701473	58.242445
H	50.930629	4.445321	58.845710	H	50.789858	4.188641	59.018763	H	51.097444	4.591928	58.696446
H	53.408769	3.724486	60.536387	H	53.562569	3.970271	60.353918	H	53.243433	3.591815	60.673906
H	51.842339	4.228298	61.174798	H	52.014156	3.909032	61.187442	H	51.785177	4.478744	61.125606
H	52.111544	6.459618	60.008814	H	51.553173	6.294024	60.435863	H	52.575284	6.456533	59.787774
H	53.741599	5.970599	59.509914	H	53.205138	6.361109	59.792334	H	54.053087	5.575564	59.364356
H	54.353929	5.616888	61.936950	H	54.090087	5.731976	62.081966	H	54.644259	5.395771	61.801723
H	52.709423	6.092755	62.405026	H	52.420062	5.686429	62.690581	H	53.124450	6.206800	62.224573
H	54.750730	7.855016	61.160340	H	53.879018	8.090987	61.733528	H	55.449479	7.418793	60.845648
H	54.069778	7.932634	62.710572	H	53.351729	7.755597	63.304451	H	54.769769	7.757505	62.365156
H	57.552293	10.840359	66.923233	H	57.636877	10.528112	66.993744	H	59.650515	10.630365	61.978165
H	51.344962	10.662452	65.346436	H	51.356455	11.129018	65.904247	H	56.847327	10.719386	67.722671
H	52.964690	10.585360	59.192715	H	52.368760	10.218732	59.670090	H	51.160868	9.830252	64.923462
H	59.119864	10.109316	60.788945	H	58.660303	10.080525	60.689247	H	53.898059	10.396511	59.184111
H	56.324894	10.802727	68.858099	H	56.531993	10.455537	69.047900	H	61.195641	9.996434	63.763777
H	54.985814	9.644190	68.564793	H	55.043887	9.466483	68.864866	H	60.337413	9.097622	65.080814
H	54.684120	11.163213	69.429282	H	54.998040	11.003843	69.747804	H	61.429359	10.438961	65.464760
H	55.058200	13.455342	66.466529	H	55.355725	13.262715	66.758870	H	59.178310	13.190875	64.166509
H	54.522724	13.389118	68.139667	H	54.940176	13.245738	68.470975	H	60.567677	12.902724	65.209001
H	52.667226	11.599279	67.485821	H	52.894929	11.681938	67.950212	H	59.201121	11.379139	66.878773
H	51.340877	7.877310	62.952503	H	50.726345	8.249494	63.961167	H	54.874205	7.679950	67.103695
H	49.677615	8.313726	62.491215	H	49.110789	8.887405	63.532053	H	54.100212	7.864162	68.704187
H	50.240026	8.565304	64.169541	H	49.842939	9.287006	65.108189	H	55.795095	8.386456	68.456258
H	50.121929	12.046399	62.719235	H	50.200536	12.503487	63.220758	H	53.955124	11.667727	68.566210
H	49.682289	11.092744	64.139159	H	49.667931	11.789121	64.741879	H	55.292530	10.760060	69.261430
H	50.772071	10.069488	60.482751	H	50.258942	10.092157	61.199698	H	52.045158	9.438991	67.376188
H	55.212956	10.541757	57.842776	H	54.472684	10.032605	58.143101	H	50.272073	10.089608	62.500683
H	57.822541	10.245478	58.537351	H	57.150301	9.933702	58.587485	H	51.420087	10.362190	60.054247
H	60.461424	10.019231	63.053304	H	60.209684	10.052277	62.839138	H	56.381894	10.095473	58.315116
H	59.760480	10.181742	65.677285	H	59.729420	10.054440	65.524593	H	58.820795	10.073976	59.527749
H	52.430373	12.786547	62.375589	H	52.447526	12.802512	62.302468	H	52.782986	12.904738	61.964407
H	53.749273	13.143391	64.519380	H	53.479919	13.121087	64.621639	H	53.124222	12.602810	64.458975
H	54.429721	14.626994	63.848585	H	54.300153	14.570003	64.034663	H	53.673374	14.281497	64.581683
H	50.529863	7.483573	69.039146	H	50.539775	7.434006	68.974997	H	52.123742	8.410082	71.216396
H	56.268739	2.929548	65.287026	H	56.360821	2.802217	65.177995	H	56.412495	2.450550	64.975905
H	57.380246	6.665864	64.160263	H	57.323898	6.637060	64.164810	H	58.930295	7.510157	63.590744
H	53.166396	8.281674	61.344910	H	52.270205	8.085588	62.062990	H	53.986719	8.177915	60.946763

H	52.040921	14.345601	63.128228	H	51.998941	14.359373	63.031196	H	51.810973	14.066337	62.898485
H	53.120627	14.280772	61.714921	H	53.248674	14.289754	61.769467	H	53.314983	14.594117	62.102744
O	54.064547	8.052360	64.509788	O	53.752255	7.950645	65.006216	O	54.460586	7.625013	64.151983
H	54.530756	8.915735	64.710065	H	54.216450	8.835945	65.072271	H	54.762673	8.479538	64.564630
H	53.128893	8.316884	64.661263	H	53.017428	8.036292	65.668464	H	53.488035	7.732631	64.194100
O	56.265172	7.800932	67.085334	O	56.240180	7.589334	67.164098	O	57.717475	7.743054	64.929244
H	56.448565	8.700305	66.713836	H	56.424734	8.496591	66.802319	H	57.360583	8.636183	64.678871
H	56.865271	7.749115	67.853049	H	56.855130	7.512672	67.917553	H	58.132042	7.895993	65.798676
H	52.129119	1.233807	63.702361	H	52.038045	1.286518	63.801428	H	52.056527	1.215995	63.612680

Heme (Fe²⁺) without NO₂⁻

S=0			S=1			S=2					
C	50.331000	-52.045950	49.409000	C	50.331000	-52.045950	49.409000	C	50.331000	-52.045950	49.409000
C	50.203228	-50.618862	48.883639	C	50.520576	-50.591588	48.980342	C	50.259044	-50.653773	48.793980
C	51.427466	-49.783026	49.237149	C	51.816409	-50.000361	49.526892	C	51.532457	-49.867686	49.075537
N	51.247922	-48.408001	48.771288	N	51.976330	-48.624255	49.047995	N	51.395067	-48.495882	48.588920
C	52.044331	-47.388613	49.097435	C	52.992285	-47.816947	49.354382	C	52.183529	-47.487441	48.959896
N	53.165575	-47.595763	49.792516	N	53.953886	-48.225807	50.188894	N	53.297858	-47.714188	49.657104
N	51.761877	-46.145346	48.657578	N	53.102615	-46.605055	48.776598	N	51.894844	-46.228340	48.565301
C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410	C	52.225000	-47.068010	42.455410
C	53.250554	-47.270179	43.573955	C	53.537828	-47.245504	43.219361	C	53.304789	-47.274729	43.520563
C	52.605986	-47.333408	44.965843	C	53.293837	-47.722146	44.656020	C	52.723750	-47.414481	44.934016
N	53.516745	-47.879272	45.981882	N	54.501397	-48.202282	45.330086	N	53.702650	-47.938087	45.896663
C	54.532342	-47.212621	46.555002	C	55.450939	-47.426516	45.870307	C	54.699952	-47.228959	46.451361
N	54.490720	-45.890133	46.722349	N	55.266920	-46.120881	46.059341	N	54.594913	-45.913354	46.642132
N	55.611728	-47.898170	46.963153	N	56.628577	-47.978739	46.210219	N	55.822391	-47.863542	46.821084
C	57.624000	-44.932480	42.491060	C	57.624000	-44.932480	42.491060	C	57.624000	-44.932480	42.491060
C	57.584000	-43.404240	42.750400	C	57.584000	-43.404240	42.750400	C	57.584000	-43.404240	42.750400
C	57.764347	-43.073118	44.242205	C	57.706060	-43.044912	44.240014	C	57.749214	-43.063413	44.240759
C	59.175539	-43.382449	44.733492	C	59.055075	-43.470686	44.806837	C	59.158587	-43.363657	44.741115
N	59.249677	-43.357831	46.231363	N	59.131802	-43.236266	46.281903	N	59.232303	-43.288178	46.237043
C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430	C	51.838000	-42.751710	40.914430
C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930	C	52.531000	-43.413060	42.112930
C	53.163418	-42.459627	43.118171	C	52.577434	-42.540784	43.379754	C	53.092921	-42.439364	43.144512
C	54.159796	-43.248920	43.947057	C	54.002520	-42.196678	43.791653	C	54.151818	-43.158999	43.957787
N	54.543812	-42.500188	45.178029	N	54.008429	-41.750965	45.214785	N	54.508007	-42.386367	45.184454
Fe	54.840344	-41.906206	48.898351	Fe	55.403854	-41.172045	48.309457	Fe	54.826987	-41.962850	49.021558
C	57.498564	-43.463807	50.286294	C	57.602555	-42.899643	50.208296	C	57.561679	-43.646171	50.228441
C	52.661686	-43.907415	50.624261	C	52.861956	-43.278035	49.155114	C	52.751476	-44.106215	50.699770
C	52.127767	-40.372239	47.364000	C	53.204654	-39.076005	46.731705	C	52.088744	-40.482475	47.523727
C	56.954486	-40.147458	46.820559	C	58.003877	-39.704272	46.550766	C	56.896192	-40.117711	46.954609
N	55.055251	-43.487497	49.985176	N	55.307990	-42.837904	49.368187	N	55.120941	-43.693300	50.049271
C	56.246967	-44.017968	50.434495	C	56.304911	-43.327270	50.209719	C	56.323256	-44.218532	50.428594
C	56.053198	-45.327732	51.190445	C	55.810715	-44.469927	51.099063	C	56.154802	-45.534756	51.185596
C	56.515623	-46.509598	50.294651	C	56.539229	-45.799239	50.792220	C	56.591429	-46.704494	50.263161
C	56.741589	-45.385078	52.583406	C	55.895034	-44.116089	52.607958	C	56.886085	-45.603356	52.556188
C	58.206444	-45.896692	52.664151	C	57.268615	-44.103981	53.337983	C	58.355217	-46.112396	52.576538
O	59.018622	-45.581341	51.740105	O	58.314670	-44.469565	52.722367	O	59.138436	-45.756589	51.643119
O	58.473614	-46.586745	53.685233	O	57.198427	-43.730258	54.541030	O	58.652385	-46.844538	53.559168
C	54.563801	-45.322405	51.324912	C	54.374001	-44.526338	50.669736	C	54.666797	-45.536718	51.365104
C	54.037020	-44.258556	50.640927	C	54.134173	-43.569208	49.720054	C	54.127852	-44.462272	50.704815
N	52.810440	-42.117023	48.985363	N	53.441134	-41.191327	48.031879	N	52.866609	-42.222488	49.134746
C	52.117476	-42.894794	49.897579	C	52.548792	-42.121748	48.488335	C	52.197129	-43.068582	50.017972
C	50.634172	-42.523167	49.970305	C	51.097641	-41.738128	48.194351	C	50.704265	-42.739025	50.107001
C	49.712445	-43.707727	49.613380	C	50.400481	-42.740328	47.246041	C	49.810910	-43.932259	49.703130
C	50.295634	-42.004778	51.394543	C	50.305879	-41.650058	49.526041	C	50.343377	-42.286691	51.547867
C	48.834285	-41.539850	51.626218	C	48.822631	-41.212036	49.415936	C	48.868558	-41.863168	51.783615
O	48.494949	-41.484726	52.842226	O	48.125518	-41.486479	50.433973	O	48.519614	-41.853506	52.997774
O	48.130098	-41.239217	50.620743	O	48.442983	-40.622729	48.364916	O	48.164033	-41.548467	50.782669

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C 54.998749 -39.285729 45.552419 C 56.397316 -38.258217 45.319182 C 54.920227 -39.189551 45.745058
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C 58.932272 -40.932654 48.158513 C 59.637484 -40.780909 48.112668 C 58.873853 -40.922404 48.264390
C 59.080529 -41.845954 49.185218 C 59.513996 -41.651528 49.175932 C 59.052738 -41.892934 49.231202
C 57.791116 -42.400248 49.439144 C 58.127803 -41.974015 49.296432 C 57.782159 -42.498608 49.465181
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C 53.704783 -40.224300 51.450997 C 53.964051 -40.137985 51.037849 C 53.601140 -40.213592 51.590747
S 55.234872 -40.528421 50.513976 S 55.391332 -39.788895 49.947663 S 55.214454 -40.574272 50.815435
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H 52.331173 -50.214695 48.778935 H 52.679781 -50.600609 49.198123 H 52.397803 -50.352174 48.598033
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H 53.332336 -48.499270 50.218406 H 53.850865 -49.080579 50.720436 H 53.501001 -48.646384 49.996198
H 52.147161 -45.349113 49.193782 H 53.673198 -45.892562 49.274076 H 52.287557 -45.461241 49.132640
H 50.818302 -45.983143 48.320891 H 52.283014 -46.240506 48.304007 H 50.934122 -46.053376 48.287442
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H 51.602987 -46.180583 42.631927 H 51.552129 -46.367306 42.967835 H 51.580627 -46.211871 42.693721
H 54.001431 -46.466318 43.562923 H 54.109611 -46.305739 43.233732 H 54.026409 -46.443656 43.508989
H 53.798730 -48.208204 43.403614 H 54.166155 -47.989890 42.709577 H 53.877830 -48.185104 43.290827
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H 57.527736 -42.017588 44.443305 H 57.574921 -41.961345 44.384244 H 57.512630 -42.005232 44.428961
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H 59.168360 -42.402159 46.639471 H 59.076915 -42.225456 46.532570 H 59.122351 -42.324668 46.612844
H 60.135217 -43.745985 46.569676 H 60.015394 -43.580224 46.669457 H 60.128642 -43.639346 46.588143
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H 53.311766 -44.089297 41.728557 H 53.554763 -43.696301 41.823290 H 53.352129 -44.043481 41.733817
H 51.814229 -44.054031 42.646441 H 52.019172 -44.353762 42.344305 H 51.833251 -44.095856 42.618194
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H 55.465932 -42.769790 45.535889 H 54.901547 -41.344573 45.556965 H 55.456859 -42.583939 45.517857

H	52.491212	-44.089962	46.902086	H	52.527165	-44.201091	47.243241	H	52.615965	-44.179127	46.975734
O	55.784362	-45.752389	48.817299	O	55.893362	-45.931889	48.867528	O	57.564096	-44.265134	47.519566
H	55.476829	-44.849739	49.062312	H	55.632398	-45.034287	49.186179	H	57.188428	-43.389864	47.820232
H	56.578150	-45.863171	49.376602	H	56.703347	-46.113227	49.384208	H	57.939107	-44.604631	48.361243
H	52.042534	-48.014759	41.929524	H	52.114077	-47.991271	41.870954	H	51.664451	-47.961556	42.761619

Table S10. Cartesian coordinates (Å) of the ligands optimized at DFT (BP86 functional) using TZ2P basis sets.

HSO ₃ ⁻			SO ₃ ²⁻			NO ₂ ⁻					
S	-1.003479	0.582431	-0.449054	S	-1.028630	0.625832	-0.307931	N	0.000000	0.000000	-1.751411
O	-1.305684	1.179513	1.193932	O	-1.338123	1.240048	1.090069	O	1.075220	0.000000	-1.062565
H	-2.202889	0.834886	1.378925	O	-2.217503	-0.330711	-0.621951	O	-1.075220	0.000000	-1.062565
O	-2.172122	-0.359413	-0.606265	O	-1.152233	1.801585	-1.322470				
O	-1.192430	1.819602	-1.278879								

Table S11. Cartesian coordinates (Å) of the Cub-Siro-Fe^{2+/3+} complexes optimized at DFT (BP86 functional) using TZ2P basis sets.

Cub-Siro-Fe ²⁺ -HSO ₃ ⁻			
Atom	X	Y	Z
C	50.372856	4.343387	71.657038
C	51.307763	5.531856	71.411271
C	51.401943	5.889023	69.929353
N	52.277232	7.045851	69.732642
C	52.775394	7.438258	68.551577
N	52.463540	6.751845	67.438757
N	53.577474	8.503436	68.468232
C	52.284463	2.213803	63.378748
C	53.744039	2.584415	63.605946
C	54.084707	2.659679	65.098725
N	55.403934	3.226502	65.364307
C	55.673780	4.528514	65.163767
N	54.689426	5.371186	64.867238
N	56.933918	4.983474	65.227952
C	57.687141	3.612576	61.777041
C	57.649484	4.793301	60.772628
C	57.512660	6.172739	61.440485
C	58.802723	6.700439	62.057964
N	58.578221	8.037176	62.696435
C	51.906989	3.806659	59.080477
C	52.597297	4.299916	60.358836
C	53.195845	5.705510	60.227940
C	53.750658	6.187148	61.560221
N	54.450400	7.500711	61.456790
Fe	55.436097	11.469765	64.261460
C	58.554462	11.268340	65.688366
C	54.074139	12.132161	67.262657
C	52.378180	10.179852	63.178283

C	56.801168	10.813884	61.155400
N	56.203890	11.608585	66.194945
C	57.513809	11.427868	66.574020
C	57.599810	11.486907	68.104059
C	57.270033	10.105987	68.718974
C	58.887546	12.071616	68.689008
C	60.149727	11.196381	68.790760
O	60.999990	11.544408	69.641665
O	60.317901	10.191443	68.000400
C	56.369647	12.389792	68.382856
C	55.467193	12.051840	67.235178
N	53.538007	11.123295	65.103488
C	53.189113	11.627701	66.317361
C	51.674402	11.586012	66.513775
C	51.235798	11.227997	67.933583
C	51.112922	12.974666	66.087610
C	49.566338	13.004796	66.133434
O	49.027876	13.524400	67.151930
O	48.961135	12.474560	65.148807
C	51.284442	10.513370	65.469896
C	52.435517	10.563944	64.499530
N	54.722368	10.577241	62.484932
C	53.409369	10.312906	62.203748
C	53.238176	10.192121	60.783152
C	54.489008	10.399886	60.207714
C	55.411378	10.622847	61.277199
N	57.346052	11.115880	63.531094
C	57.708013	11.024134	62.194967
C	59.148259	11.083120	62.100621
C	59.631248	11.166089	63.389362
C	58.490407	11.192390	64.275467
S	55.916868	8.651906	65.093753
O	57.435140	7.846547	65.130443
O	55.345532	7.817932	63.938608
O	55.274859	8.184705	66.361511
C	52.899647	13.711517	62.671869
C	53.736770	14.426066	63.715864
S	55.480198	13.813515	63.706158
H	54.891203	6.361062	64.607443
H	50.328183	4.102983	72.725584

H	50.721335	3.448389	71.123796
H	49.351819	4.564320	71.318076
H	50.953345	6.409840	71.971166
H	52.315172	5.292017	71.781502
H	51.813394	5.032088	69.374410
H	50.398474	6.105714	69.528929
H	52.651467	7.139844	66.503897
H	51.694406	6.095524	67.487337
H	54.163045	8.618595	67.623889
H	53.900946	8.947317	69.319639
H	52.066589	2.100584	62.310815
H	51.616317	2.989785	63.776825
H	53.942374	3.562672	63.145779
H	54.434465	1.883389	63.116334
H	54.070705	1.659780	65.545926
H	53.324378	3.241844	65.642860
H	53.724167	5.075167	64.895300
H	57.677885	4.358669	65.510747
H	57.112909	5.999381	65.265048
H	57.765906	2.656409	61.246091
H	56.770876	3.592166	62.383154
H	58.541174	3.689703	62.462188
H	58.549166	4.779627	60.140552
H	56.796124	4.653505	60.094776
H	56.737727	6.133866	62.222213
H	57.194065	6.905208	60.680847
H	59.577430	6.818919	61.293496
H	59.186746	6.037391	62.840393
H	58.022458	8.677618	62.103182
H	59.458151	8.542078	62.868968
H	51.502799	2.795897	59.218374
H	52.610682	3.777323	58.237233
H	51.076044	4.468957	58.802486
H	53.395004	3.596569	60.643334
H	51.872369	4.298501	61.186894
H	52.428457	6.410590	59.874852
H	53.996228	5.699342	59.471016
H	54.480029	5.473387	61.965375
H	52.961789	6.315159	62.310802
H	55.227237	7.455958	60.790643

H	54.838146	7.795064	62.402340
H	59.549542	11.204945	66.122267
H	53.639212	12.554469	68.165647
H	51.402648	9.870018	62.802804
H	57.207434	10.794782	60.143499
H	58.063846	9.379878	68.538987
H	56.339273	9.710642	68.293576
H	57.142066	10.220427	69.803872
H	59.161742	12.971207	68.113794
H	58.677447	12.427738	69.707093
H	55.921836	12.237441	69.370509
H	51.705991	10.290651	68.256042
H	50.145417	11.114390	67.971694
H	51.502992	12.018839	68.645444
H	51.442718	13.182420	65.061437
H	51.527650	13.742098	66.753368
H	51.240332	9.525026	65.957352
H	52.290983	10.030226	60.275228
H	54.740130	10.398098	59.150562
H	59.718847	11.050444	61.176172
H	60.667262	11.235764	63.709048
H	59.383000	7.602811	67.332610
H	52.802648	12.647866	62.902240
H	53.334233	14.284812	64.725694
H	53.793758	15.505120	63.524887
H	52.548548	7.575750	70.554350
H	56.171589	2.605002	65.589806
H	58.087108	7.957758	63.644482
H	53.832249	8.280084	61.130618
H	51.889055	14.144328	62.637022
H	53.349965	13.804869	61.674882
O	52.340229	7.340566	64.603142
H	52.649938	8.218618	64.274645
H	51.373105	7.399238	64.507161
O	59.309918	8.321632	66.683300
H	58.142728	8.183050	65.865336
H	59.608312	9.185867	67.200246
H	52.029520	1.265733	63.872427
Fe	55.297778	17.838325	66.756132
Fe	57.038764	15.979613	68.074732

Fe	56.123685	15.308999	65.446834
Fe	57.962915	17.202843	65.644882
S	58.281635	14.945117	66.360242
S	55.865297	17.483831	64.485731
S	57.440330	18.304784	67.696831
S	54.765354	15.595830	67.358090
C	56.655012	17.001310	71.047094
S	57.336347	15.465638	70.287364
C	54.140446	21.081532	66.954506
S	53.625791	19.337121	67.305183
C	58.784509	19.947189	64.543863
S	59.560046	18.277837	64.394462
H	55.596425	17.111629	70.787278
H	57.204504	17.874889	70.680995
H	53.364922	21.745693	67.350285
H	55.096592	21.297795	67.443375
H	58.733511	20.246906	65.596539
H	56.758175	16.924901	72.135603
H	57.770074	19.921496	64.129375
H	59.392149	20.668202	63.984604
H	54.240838	21.234051	65.874462
H	56.647097	13.455459	68.301419
H	50.313969	10.728976	65.007907

Cub-Siro-Fe ²⁺ -SO ₃ ²⁻			
Atom	X	Y	Z
C	50.420085	4.269092	71.532002
C	51.773900	4.981888	71.496789
C	51.863033	6.016198	70.371698
N	53.127047	6.747843	70.453496
C	53.968976	6.964276	69.438152
N	53.626029	6.771413	68.166229
N	55.247471	7.333781	69.691001
C	52.314085	2.142092	63.249002
C	53.795562	2.448924	63.378888
C	54.366006	2.052095	64.747131
N	55.671344	2.664131	64.999795
C	55.760885	4.016744	65.087914
N	54.682270	4.713476	65.441079
N	56.903990	4.649677	64.839427

C	57.713085	3.542092	61.636002
C	57.673085	4.723092	60.632002
C	57.545368	6.090296	61.316747
C	58.809066	6.530399	62.054761
N	58.595423	7.849777	62.704341
C	51.927085	3.736092	58.952002
C	52.620085	4.229092	60.229003
C	52.486899	5.705238	60.629705
C	53.260976	5.915516	61.934345
N	53.160195	7.278827	62.522308
Fe	55.035432	10.984610	64.760653
C	58.172708	10.645198	63.420200
C	56.415300	11.597602	67.809905
C	51.929891	10.651096	66.233067
C	53.636713	10.162741	61.670920
N	56.985410	11.017147	65.507123
C	58.121319	10.726500	64.789002
C	59.289187	10.522697	65.749715
C	59.261892	9.068419	66.283297
C	60.676503	10.882870	65.203707
C	61.447992	9.857939	64.334000
O	60.817735	9.001653	63.612854
O	62.700434	9.951934	64.364764
C	58.816500	11.439705	66.907462
C	57.314192	11.359973	66.771873
N	54.286395	11.031269	66.749483
C	55.036349	11.395406	67.816838
C	54.189210	11.557248	69.081752
C	54.741377	10.715151	70.237172
C	54.133893	13.052346	69.484706
C	53.214716	13.265737	70.708378
O	53.765417	13.298250	71.848894
O	51.967092	13.355235	70.480623
C	52.807572	11.050432	68.596945
C	52.970871	10.892742	67.107530
N	53.126505	10.455593	64.072587
C	51.984716	10.465439	64.825980
C	50.845775	10.241483	63.974799
C	51.322474	10.100236	62.686579
C	52.751938	10.242928	62.752019

N	55.770396	10.448474	62.871273
C	55.033724	10.267408	61.714339
C	55.927122	10.232316	60.590293
C	57.204794	10.418533	61.085943
C	57.086063	10.555716	62.515148
S	55.594590	8.120760	65.326193
O	56.687816	7.356280	64.553049
O	54.265611	7.319609	64.923561
O	55.790759	7.744643	66.804215
C	52.926085	13.640092	62.544002
C	53.283424	13.849280	64.005332
S	55.019112	13.326880	64.317648
H	54.604535	5.751613	65.291237
H	50.389326	3.536367	72.347585
H	50.228239	3.735542	70.590747
H	49.599636	4.982935	71.687442
H	51.952706	5.486168	72.458656
H	52.579424	4.245478	71.361709
H	51.819044	5.522208	69.393420
H	51.021391	6.722128	70.428076
H	54.360350	7.064292	67.486561
H	52.668020	6.905620	67.823019
H	55.722017	7.848492	68.946515
H	55.525237	7.545818	70.642006
H	51.914031	2.412789	62.268777
H	51.740267	2.682242	64.014975
H	53.935261	3.534132	63.275338
H	54.417380	2.016626	62.582219
H	54.497562	0.966248	64.821736
H	53.670826	2.317412	65.556500
H	53.839719	4.218731	65.697711
H	57.697001	4.132619	64.483953
H	56.916416	5.698891	64.835113
H	57.787076	2.581714	61.110334
H	56.797097	3.527298	62.242036
H	58.576241	3.614472	62.311124
H	58.575116	4.706925	60.002189
H	56.817674	4.585718	59.955903
H	56.708465	6.072491	62.033727
H	57.300296	6.857917	60.566927

H	59.654736	6.622053	61.363239
H	59.096885	5.823090	62.840535
H	58.223517	8.528896	62.024179
H	59.477536	8.296688	63.127051
H	52.116215	2.664356	58.813280
H	52.295997	4.263988	58.061562
H	50.839443	3.885386	59.003262
H	53.694614	3.992949	60.154656
H	52.247415	3.631233	61.067847
H	51.428663	5.967932	60.781170
H	52.881798	6.366915	59.844661
H	54.330205	5.717359	61.786240
H	52.896600	5.224489	62.703010
H	53.554992	8.024236	61.920634
H	53.680806	7.345143	63.481142
H	59.164715	10.547114	62.984264
H	56.855330	11.927770	68.749791
H	50.930184	10.644419	66.670501
H	53.187123	10.045095	60.683020
H	59.459700	8.348859	65.484986
H	58.288682	8.834875	66.732423
H	60.039571	8.955138	67.051839
H	60.608512	11.811836	64.615069
H	61.336516	11.114284	66.050243
H	59.182503	11.126939	67.892263
H	54.819060	9.667040	69.933966
H	54.076566	10.787355	71.106513
H	55.733170	11.065316	70.549212
H	53.763848	13.639059	68.634520
H	55.146924	13.405778	69.717819
H	52.558374	10.079198	69.053675
H	49.812863	10.206111	64.311054
H	50.749352	9.938797	61.776982
H	55.626375	10.104700	59.553773
H	58.133743	10.484874	60.524754
H	53.085466	12.599690	62.247859
H	52.640976	13.261062	64.671151
H	53.201393	14.904658	64.295872
H	53.445456	7.009470	71.381537
H	56.493535	2.169003	64.672485

H	57.860347	7.779370	63.461482
H	52.186202	7.559911	62.694476
H	51.869823	13.893075	62.365656
H	53.546440	14.280175	61.902476
O	51.847312	7.505646	66.123400
H	52.744440	7.501875	65.683296
H	51.677626	8.467817	66.220594
O	57.099139	5.565851	67.917948
H	56.712307	6.307462	67.383281
H	56.755147	5.746257	68.810821
H	52.112459	1.070083	63.391897
Fe	55.104391	17.826000	66.349854
Fe	56.769932	15.993527	67.921252
Fe	55.834434	15.111137	65.590469
Fe	57.802120	17.100394	65.487317
S	58.106359	14.912490	66.253177
S	55.776792	17.066510	64.192437
S	57.151133	18.319427	67.446944
S	54.431368	15.811252	67.344278
C	56.699085	16.928092	70.912002
S	57.355273	15.423764	70.059486
C	54.175085	21.009092	66.826002
S	53.395999	19.373444	66.477606
C	58.814085	19.876092	64.405002
S	59.507574	18.168661	64.377419
H	55.606503	16.871556	70.969363
H	56.989576	17.829739	70.361297
H	53.471300	21.616642	67.406061
H	55.100047	20.875263	67.398729
H	58.617508	20.181699	65.438834
H	57.114019	16.962867	71.925880
H	57.875831	19.909756	63.839476
H	59.539573	20.560373	63.949520
H	54.406204	21.519606	65.884118
H	59.118814	12.487281	66.736133
H	52.011805	11.754484	68.872798

Cub-Siro-Fe²⁺-NO₂⁻

Atom	X	Y	Z
C	50.331000	4.395000	71.629000

C	50.576952	5.363569	70.456940
C	52.054776	5.704866	70.220324
N	52.189208	6.552100	69.026740
C	53.343804	7.054295	68.538052
N	54.517290	6.755274	69.089478
N	53.290252	7.877477	67.473697
C	52.014676	2.386622	63.403636
C	53.476432	2.726647	63.647583
C	53.912488	2.437561	65.089847
N	55.206979	3.036002	65.415199
C	55.359960	4.376131	65.428839
N	54.295038	5.175654	65.534999
N	56.565376	4.942657	65.347585
C	57.527496	3.689662	61.815396
C	57.508096	4.862472	60.801236
C	57.186717	6.194503	61.505247
C	58.304050	6.711556	62.406820
N	57.893415	7.957533	63.120170
C	51.593946	3.987472	59.112356
C	52.310056	4.470472	60.380396
C	52.935926	5.863386	60.318826
C	53.419789	6.228370	61.714440
N	54.156745	7.513813	61.796570
Fe	54.722338	11.026331	64.750618
C	57.552706	10.759604	66.595440
C	53.076981	12.287961	67.340753
C	51.802436	10.157384	63.222552
C	56.439305	10.868018	61.854756
N	55.198620	11.315154	66.651671
C	56.393489	11.012959	67.276953
C	56.246022	11.260095	68.779317
C	55.495634	10.125675	69.513273
C	57.541484	11.621672	69.498608
C	58.560209	10.491741	69.774925
O	58.432725	9.361076	69.188199
O	59.491536	10.781227	70.568234
C	55.240328	12.439340	68.689544
C	54.426467	12.036731	67.505513
N	52.788411	11.054960	65.260862
C	52.303044	11.693442	66.358434

C	50.783500	11.702011	66.378437
C	50.199651	11.415532	67.762773
C	50.321460	13.084656	65.837670
C	48.775336	13.172926	65.748684
O	48.185747	13.801973	66.670951
O	48.234219	12.582446	64.763906
C	50.472421	10.587594	65.354695
C	51.728078	10.537074	64.533508
N	54.222962	10.524345	62.889474
C	52.958494	10.276496	62.415674
C	52.981348	10.229800	60.984985
C	54.289441	10.482341	60.593687
C	55.059744	10.646918	61.782753
N	56.632626	10.849026	64.305529
C	57.175299	10.954633	63.028506
C	58.606575	11.028076	63.139947
C	58.917844	10.908274	64.476419
C	57.675915	10.819952	65.195419
N	55.237388	8.299015	65.179840
O	56.468405	7.725702	65.256867
O	54.435132	7.535230	64.344369
C	52.650586	13.550772	62.708276
C	53.393260	14.230706	63.842259
S	55.002304	13.403407	64.171428
H	54.363740	6.145974	65.108893
H	49.257698	4.199097	71.736283
H	50.697944	4.813867	72.575867
H	50.837010	3.433938	71.462975
H	50.165428	4.933535	69.531540
H	50.032917	6.301042	70.647405
H	52.464643	6.223955	71.102059
H	52.637729	4.782959	70.069412
H	55.416367	7.113128	68.673025
H	54.547194	6.290581	69.988382
H	54.167921	8.158702	67.015969
H	52.517749	7.778045	66.798952
H	51.720913	2.599327	62.371056
H	51.364003	2.970019	64.069257
H	53.622415	3.799517	63.457128
H	54.155523	2.211008	62.954026

H	54.002599	1.359758	65.263513
H	53.156135	2.792864	65.805462
H	53.374727	4.756649	65.566472
H	57.400109	4.379139	65.263585
H	56.615510	5.986506	65.382000
H	57.693319	2.731529	61.307829
H	56.568714	3.629281	62.349584
H	58.324361	3.811884	62.559881
H	58.472455	4.935394	60.278917
H	56.742191	4.675183	60.037186
H	56.289922	6.047444	62.127861
H	56.965917	6.968529	60.751506
H	59.202640	6.929833	61.818618
H	58.570741	5.979280	63.176204
H	57.451028	8.640572	62.486845
H	58.706512	8.454930	63.506424
H	51.181888	2.981744	59.262609
H	52.280397	3.947523	58.255178
H	50.764835	4.657816	58.847979
H	53.094720	3.746732	60.651674
H	51.588014	4.460700	61.211653
H	52.200377	6.605660	59.974651
H	53.774860	5.880559	59.605829
H	54.094102	5.453492	62.104000
H	52.578035	6.307428	62.413606
H	55.008422	7.492133	61.230048
H	54.405474	7.681912	62.863631
H	58.457560	10.587982	67.170330
H	52.577378	12.875834	68.105754
H	50.876070	9.872979	62.725855
H	56.978576	10.968980	60.913289
H	56.116190	9.236603	69.615677
H	54.567289	9.863312	68.989932
H	55.230383	10.484180	70.517025
H	58.068217	12.408292	68.936231
H	57.291846	12.073461	70.468694
H	54.662507	12.615039	69.601507
H	50.624914	10.491499	68.176805
H	49.110579	11.303125	67.691098
H	50.398216	12.237031	68.461275

H	50.744836	13.229512	64.834809
H	50.703973	13.870831	66.500081
H	50.321750	9.633479	65.886354
H	52.109770	10.085729	60.353451
H	54.682714	10.540856	59.583120
H	59.288698	11.139353	62.301889
H	59.898609	10.926891	64.941260
H	52.290746	12.563817	63.002562
H	52.812869	14.229570	64.772954
H	53.636597	15.273994	63.600337
H	51.336688	6.966596	68.663136
H	56.039656	2.464045	65.331997
H	57.203798	7.807437	64.004822
H	53.592459	8.319016	61.458183
H	51.777348	14.153662	62.419427
H	53.294163	13.434270	61.826666
O	51.889194	7.417890	65.016126
H	52.847893	7.569096	64.732448
H	51.428133	8.178455	64.616049
O	56.891344	7.581144	67.943378
H	56.812098	7.791684	66.976624
H	57.410636	8.337199	68.358004
H	51.811992	1.322997	63.593074
Fe	54.924292	17.789435	66.395682
Fe	56.428312	15.904997	68.159318
Fe	55.712077	14.997104	65.740084
Fe	57.757876	17.018013	65.819239
S	57.908768	14.810246	66.594045
S	55.859380	16.976241	64.359068
S	56.841195	18.207848	67.712120
S	54.159097	15.751438	67.328641
C	56.384436	16.838522	71.093916
S	56.622832	15.189543	70.312200
C	53.777736	20.906312	67.046846
S	53.320836	19.388168	66.100132
C	58.430386	19.876242	64.606136
S	59.373898	18.315408	64.874439
H	55.445486	17.289953	70.754899
H	57.214606	17.504958	70.839590
H	52.905822	21.231342	67.624080

H	54.611348	20.697094	67.725655
H	58.070639	20.258937	65.567237
H	56.344742	16.699967	72.180589
H	57.573328	19.682826	63.952432
H	59.098082	20.608427	64.139594
H	54.068465	21.693579	66.343308
H	55.773697	13.373494	68.437387
H	49.575775	10.813704	64.767110

Cub-Siro-Fe³⁺-HSO₃⁻

Atom	X	Y	Z
C	50.371954	4.344128	71.656461
C	51.588346	5.241150	71.432264
C	51.705401	5.656656	69.970732
N	52.866735	6.522942	69.776248
C	53.292734	6.955327	68.583208
N	52.649431	6.594152	67.468391
N	54.362979	7.764115	68.505615
C	52.284255	2.214920	63.378235
C	53.776794	2.439895	63.584796
C	54.174367	2.354563	65.063819
N	55.545538	2.794952	65.313997
C	55.909780	4.084241	65.204907
N	54.970083	5.013936	65.030144
N	57.197224	4.441136	65.256444
C	57.687124	3.613611	61.777097
C	57.649595	4.794390	60.772743
C	57.874485	6.169259	61.419329
C	59.331096	6.393241	61.810394
N	59.491488	7.666330	62.579994
C	51.907225	3.808014	59.080012
C	52.597431	4.301183	60.358461
C	53.260288	5.686689	60.308050
C	53.838733	6.023966	61.682426
N	54.554017	7.341819	61.725066
Fe	55.234479	11.489098	64.356105
C	58.409964	10.925320	65.636070
C	54.208276	12.493822	67.371230
C	52.029448	10.348217	63.618694
C	56.306636	10.577491	61.250755

N	56.146295	11.568205	66.221816
C	57.428554	11.195237	66.557558
C	57.564335	11.268909	68.080439
C	56.898774	10.035549	68.738390
C	58.992766	11.469255	68.616280
C	59.696243	10.115598	68.823258
O	59.874678	9.396060	67.762159
O	59.991919	9.756213	69.983030
C	56.590349	12.446198	68.343432
C	55.564519	12.203589	67.271359
N	53.412869	11.336957	65.372637
C	53.204782	12.008149	66.535393
C	51.718645	12.172085	66.813872
C	51.338133	12.008454	68.284574
C	51.331214	13.583071	66.278311
C	49.801903	13.823746	66.353118
O	49.373500	14.481843	67.340895
O	49.108844	13.313459	65.419557
C	51.128707	11.067275	65.903945
C	52.212017	10.866688	64.880275
N	54.329053	10.555723	62.729885
C	53.000401	10.266100	62.580420
C	52.732202	9.959495	61.203358
C	53.928360	10.111589	60.513476
C	54.928969	10.458633	61.478286
N	57.046512	10.864457	63.577809
C	57.296614	10.749809	62.217313
C	58.720745	10.746595	62.011089
C	59.311393	10.819374	63.258661
C	58.251323	10.891636	64.229372
S	56.725145	8.112254	65.078121
O	57.869773	7.212018	64.606810
O	55.462048	7.607817	64.330807
O	56.429350	7.465835	66.558637
C	52.899859	13.712653	62.672016
C	53.868062	14.575834	63.452416
S	55.495118	13.741707	63.728500
H	55.213115	6.009092	64.863647
H	50.298613	4.043761	72.708500
H	50.436113	3.430404	71.049781

H	49.441090	4.862660	71.389770
H	51.519514	6.140872	72.060729
H	52.502429	4.702973	71.724580
H	51.808812	4.757543	69.342122
H	50.793832	6.189079	69.656697
H	52.780825	7.115202	66.572740
H	51.788306	6.069234	67.561784
H	54.942210	7.770895	67.655460
H	54.864101	7.973533	69.361774
H	52.028386	2.214976	62.313243
H	51.696866	3.005384	63.865217
H	54.043832	3.436767	63.206743
H	54.392322	1.734634	63.009457
H	54.100623	1.322441	65.423119
H	53.481490	2.937726	65.690751
H	53.996044	4.775850	65.158014
H	57.919975	3.733118	65.261953
H	57.475544	5.425512	65.126347
H	57.525210	2.661446	61.258053
H	56.900213	3.726840	62.534530
H	58.650173	3.551037	62.299662
H	58.394969	4.634182	59.980047
H	56.672099	4.797179	60.269067
H	57.250956	6.266175	62.321552
H	57.578329	6.966049	60.718481
H	59.976750	6.439430	60.927187
H	59.694686	5.592611	62.463050
H	59.193469	8.508268	62.058680
H	60.464820	7.819223	62.859290
H	51.476097	2.812936	59.243682
H	52.615726	3.737911	58.243400
H	51.095724	4.484145	58.778873
H	53.363809	3.566348	60.652842
H	51.859499	4.309047	61.175540
H	52.526699	6.453753	60.018952
H	54.060433	5.699838	59.551604
H	54.564254	5.264903	62.001899
H	53.051594	6.081089	62.443102
H	55.330940	7.365465	61.055898
H	54.955814	7.538518	62.683554

H	59.400751	10.711108	66.029542
H	53.893727	13.051911	68.249598
H	51.010087	10.077129	63.346363
H	56.639954	10.485012	60.216737
H	57.404485	9.107643	68.467627
H	55.848795	9.968229	68.429525
H	56.934125	10.151886	69.829212
H	59.562773	12.101339	67.921126
H	58.945026	11.987126	69.581419
H	56.180421	12.469395	69.358003
H	51.698326	11.046750	68.674193
H	50.247797	12.049367	68.394293
H	51.755650	12.815745	68.898491
H	51.649287	13.658712	65.230244
H	51.868096	14.341255	66.862070
H	50.982083	10.141245	66.483459
H	51.756287	9.715019	60.794284
H	54.100033	9.981331	59.448528
H	59.212324	10.725248	61.041396
H	60.371382	10.845283	63.493922
H	57.368455	7.379311	67.087659
H	52.593707	12.833917	63.246235
H	53.464093	14.844301	64.437484
H	54.113525	15.506267	62.927063
H	53.447071	6.720583	70.584432
H	56.266616	2.101390	65.473029
H	58.884311	7.616707	63.461758
H	53.925191	8.136391	61.466503
H	51.995063	14.291483	62.439915
H	53.341972	13.367313	61.728447
O	52.902231	7.733269	64.980367
H	53.868660	7.863857	64.787547
H	52.489411	8.593484	64.737036
O	58.640605	7.199419	67.741019
H	59.215539	8.090511	67.787621
H	58.557954	6.899907	68.662620
H	51.961226	1.251728	63.797152
Fe	55.270189	18.008934	66.203918
Fe	56.675485	16.060871	68.025754
Fe	56.098378	15.195998	65.496825

Fe	58.149460	17.208426	65.759614
S	58.238330	14.994049	66.483438
S	56.319802	17.224465	64.214640
S	57.126630	18.355366	67.625885
S	54.486354	15.920438	67.033020
C	56.654555	17.001889	71.047760
S	56.741752	15.370530	70.191457
C	54.140492	21.082405	66.955155
S	53.739010	19.647907	65.865169
C	58.784741	19.948045	64.544879
S	59.824013	18.474356	64.920115
H	55.724473	17.515224	70.781935
H	57.507395	17.624529	70.760305
H	53.202906	21.594816	67.194923
H	54.620879	20.739165	67.877569
H	58.302419	20.307022	65.460474
H	56.675277	16.819250	72.127906
H	58.016202	19.684979	63.810680
H	59.434175	20.731862	64.139261
H	54.812088	21.765902	66.424922
H	57.104395	13.401510	68.142088
H	50.171392	11.370455	65.464286

Cub-Siro-Fe³⁺-SO₃²⁻

Atom	X	Y	Z
C	50.420085	4.269092	71.532002
C	51.686487	5.125442	71.471219
C	51.629230	6.161880	70.346768
N	52.800731	7.035068	70.394907
C	53.565378	7.377350	69.349802
N	53.156957	7.196639	68.088389
N	54.777813	7.908717	69.551723
C	52.314085	2.142092	63.249002
C	53.777298	2.539316	63.352845
C	54.418630	2.147340	64.689867
N	55.689943	2.839691	64.910217
C	55.715232	4.186212	65.057417
N	54.617142	4.822485	65.469751
N	56.822639	4.882225	64.811976
C	57.713085	3.542092	61.636002

C	57.673085	4.723092	60.632002
C	57.434061	6.081916	61.299336
C	58.652101	6.604502	62.053398
N	58.382154	7.948017	62.625383
C	51.927085	3.736092	58.952002
C	52.620085	4.229092	60.229002
C	52.261675	5.633057	60.735896
C	53.206297	5.989709	61.881707
N	52.875011	7.243546	62.610807
Fe	54.940917	10.997103	64.974881
C	57.940934	10.716148	63.337118
C	56.603300	11.734027	67.858220
C	52.004316	10.690812	66.757982
C	53.261590	10.225200	62.042586
N	56.952731	11.069284	65.533469
C	58.016427	10.792908	64.705474
C	59.269920	10.608124	65.557361
C	59.282087	9.159577	66.109029
C	60.609869	10.952610	64.886597
C	61.307476	9.810693	64.112872
O	60.635617	9.152463	63.233131
O	62.516429	9.600245	64.365918
C	58.905385	11.533012	66.744038
C	57.398913	11.449603	66.752879
N	54.393570	11.115176	67.016037
C	55.228611	11.545593	67.994205
C	54.475633	11.839930	69.287478
C	55.189715	11.327713	70.540966
C	54.305278	13.375220	69.368741
C	53.518928	13.911828	70.595959
O	52.634416	13.168598	71.119014
O	53.820604	15.084766	70.954911
C	53.125489	11.138739	69.008280
C	53.123490	10.955036	67.514813
N	52.984493	10.499308	64.489368
C	51.921264	10.516131	65.355252
C	50.703804	10.322091	64.611680
C	51.058160	10.194527	63.279788
C	52.485294	10.303477	63.208535
N	55.503962	10.496562	63.016902

C	54.654262	10.324256	61.941163
C	55.433564	10.309290	60.731925
C	56.751571	10.495695	61.099514
C	56.775608	10.616355	62.536961
S	55.406170	8.308465	65.365516
O	56.586351	7.623722	64.665609
O	54.153723	7.437662	64.928800
O	55.547036	7.984159	66.858256
C	52.926085	13.640092	62.544002
C	53.185950	13.806370	64.031626
S	54.920595	13.316131	64.404091
H	54.504086	5.857004	65.341378
H	50.485983	3.535458	72.344704
H	50.267560	3.719411	70.592791
H	49.529898	4.888447	71.708326
H	51.831064	5.645009	72.430652
H	52.563672	4.481248	71.313571
H	51.616016	5.659829	69.371226
H	50.710492	6.762606	70.426634
H	53.842282	7.467495	67.367055
H	52.173178	7.188849	67.840686
H	55.309229	8.201445	68.726955
H	55.255488	7.787897	70.435108
H	51.869669	2.421759	62.290070
H	51.727261	2.623004	64.044148
H	53.848121	3.632566	63.279170
H	54.397853	2.167708	62.525209
H	54.625595	1.072168	64.732963
H	53.738349	2.350127	65.529484
H	53.791875	4.285495	65.698144
H	57.632100	4.418348	64.422002
H	56.810068	5.924528	64.889794
H	57.864859	2.588113	61.116228
H	56.764329	3.480820	62.186956
H	58.532359	3.653720	62.359681
H	58.610456	4.754628	60.057237
H	56.868882	4.539150	59.906064
H	56.580525	6.016416	61.993740
H	57.162614	6.824093	60.532928
H	59.514446	6.693500	61.382480

H	58.945823	5.949696	62.881419
H	57.959555	8.560156	61.914237
H	59.278575	8.452609	62.966177
H	52.276951	2.728358	58.696183
H	52.140948	4.396862	58.100864
H	50.836060	3.693810	59.077866
H	53.709738	4.196580	60.062361
H	52.428059	3.514706	61.035131
H	51.219268	5.658092	61.088325
H	52.353011	6.375044	59.929137
H	54.236107	6.096882	61.520838
H	53.198945	5.197420	62.637042
H	52.963612	8.098547	62.036637
H	53.520769	7.384088	63.464802
H	58.892567	10.633081	62.815030
H	57.128649	12.102360	68.737581
H	51.058524	10.637536	67.296819
H	52.711789	10.130227	61.103700
H	59.391733	8.422699	65.308468
H	58.347358	8.956072	66.645554
H	60.123805	9.047595	66.805697
H	60.466743	11.799010	64.197437
H	61.311849	11.286400	65.660112
H	59.360573	11.228016	67.693233
H	55.422490	10.259642	70.457459
H	54.539368	11.485471	71.409395
H	56.124178	11.877072	70.715106
H	53.789010	13.740344	68.467430
H	55.292170	13.857371	69.367120
H	53.097866	10.154561	69.502303
H	49.703608	10.323733	65.036801
H	50.397334	10.055467	62.428438
H	55.033058	10.195593	59.728380
H	57.619186	10.572575	60.449279
H	53.145161	12.620527	62.217610
H	52.529375	13.172663	64.637983
H	53.056308	14.846919	64.354849
H	53.136697	7.306769	71.313953
H	56.534731	2.397618	64.564799
H	57.684655	7.911123	63.413637

H	51.924611	7.224916	63.007081
H	51.872230	13.858035	62.315552
H	53.554006	14.330172	61.965852
O	51.498869	7.336809	65.382322
H	52.478173	7.506460	65.347742
H	51.114082	8.230805	65.270567
O	57.639373	6.458824	67.732881
H	56.903872	6.996572	67.336030
H	58.443280	6.863722	67.366500
H	52.184227	1.055735	63.358872
Fe	55.186660	18.014602	66.038377
Fe	56.687175	16.113426	67.910088
Fe	55.730830	15.118412	65.595737
Fe	57.925469	17.062767	65.389893
S	57.992739	14.907570	66.255812
S	55.937476	16.961190	64.046453
S	57.166570	18.382659	67.263743
S	54.387631	16.129307	67.229371
C	56.699085	16.928092	70.912002
S	57.540415	15.605190	69.938792
C	54.175085	21.009092	66.826002
S	53.763305	19.722136	65.573931
C	58.814085	19.876092	64.405002
S	59.613099	18.215631	64.412717
H	55.650173	16.636982	71.044309
H	56.773255	17.887963	70.389010
H	53.689342	20.768385	67.777710
H	55.258840	21.064113	66.975002
H	58.651072	20.211118	65.434595
H	57.195093	17.002883	71.886508
H	57.851552	19.828934	63.884191
H	59.479231	20.574344	63.884386
H	53.805548	21.973321	66.459788
H	59.191050	12.578094	66.538848
H	52.281180	11.719396	69.390910

Cub-Siro-Fe³⁺-NO₂⁻

Atom	X	Y	Z
C	50.331000	4.395000	71.629000
C	51.501030	5.387188	71.636689

C	51.705083	6.097876	70.292687
N	52.759838	7.110369	70.408956
C	53.812517	7.262937	69.596779
N	53.845428	6.700205	68.373084
N	54.872694	7.973947	70.001306
C	52.014676	2.386622	63.403636
C	53.485255	2.765262	63.517782
C	54.050918	2.528626	64.923355
N	55.360682	3.153538	65.111269
C	55.504398	4.490210	65.154416
N	54.447328	5.282576	65.316931
N	56.708635	5.066926	65.048854
C	57.527496	3.689662	61.815396
C	57.508096	4.862472	60.801236
C	57.287819	6.233550	61.479363
C	58.517157	6.747545	62.224070
N	58.262335	8.068206	62.883959
C	51.593946	3.987472	59.112356
C	52.310055	4.470472	60.380396
C	52.869185	5.894544	60.376558
C	53.421275	6.188464	61.766569
N	53.991247	7.550218	61.931038
Fe	55.303129	10.873539	64.549872
C	58.686001	11.281638	65.062232
C	54.728175	11.495554	67.842539
C	51.922153	10.253663	64.086886
C	55.803445	10.742563	61.142995
N	56.534338	11.228551	66.211582
C	57.904248	11.318549	66.196499
C	58.445162	11.472026	67.618904
C	58.798821	10.068043	68.156446
C	59.632393	12.450096	67.781669
C	61.024362	11.808177	67.603350
O	61.378771	11.461831	66.432833
O	61.718576	11.657072	68.649581
C	57.176696	11.980407	68.340818
C	56.057824	11.536036	67.444345
N	53.587835	10.768158	65.801434
C	53.602334	11.133939	67.103339
C	52.204039	11.180019	67.702452

C	52.081741	10.268765	68.929423
C	51.893905	12.660812	68.051403
C	50.429542	12.819361	68.532379
O	50.241067	12.818544	69.781062
O	49.546758	12.900013	67.626202
C	51.330979	10.685080	66.525149
C	52.300058	10.522352	65.384490
N	54.082612	10.511459	62.902109
C	52.729155	10.281322	62.926673
C	52.247993	10.162842	61.576848
C	53.334787	10.358412	60.739696
C	54.482992	10.564347	61.576487
N	56.948768	10.962248	63.320131
C	56.939900	10.925679	61.934298
C	58.290617	11.103041	61.460693
C	59.097457	11.245624	62.567864
C	58.249280	11.163650	63.728804
N	55.531819	8.614172	64.723505
O	56.665943	7.903546	64.965216
O	54.469235	7.802430	64.474267
C	52.650586	13.550772	62.708276
C	53.062538	13.615186	64.168923
S	54.883511	13.391553	64.364924
H	54.527384	6.307043	65.063390
H	50.228973	3.916170	72.609995
H	50.484066	3.604773	70.881252
H	49.383270	4.899989	71.398575
H	51.329738	6.148354	72.413267
H	52.431720	4.864254	71.900422
H	52.007620	5.386224	69.515092
H	50.770664	6.576983	69.965571
H	54.737504	6.849889	67.877945
H	53.018488	6.760777	67.765359
H	55.605443	8.176889	69.319913
H	55.008078	8.219570	70.973553
H	51.636187	2.563155	62.391517
H	51.404440	2.973053	64.104367
H	53.593934	3.832898	63.283519
H	54.109569	2.234252	62.785377
H	54.173713	1.458611	65.122681

H	53.357873	2.899754	65.693119
H	53.524187	4.885244	65.428024
H	57.525696	4.514977	64.826159
H	56.750044	6.106585	65.041189
H	57.657056	2.730793	61.299523
H	56.581632	3.648505	62.373065
H	58.350290	3.789872	62.535657
H	58.443485	4.882963	60.224638
H	56.696687	4.699535	60.079805
H	56.451746	6.151279	62.193707
H	57.009429	6.978063	60.716633
H	59.358081	6.874331	61.533716
H	58.830637	6.058339	63.015254
H	57.891923	8.766484	62.219056
H	59.134633	8.470005	63.244525
H	51.233082	2.960573	59.248013
H	52.264827	3.998731	58.242373
H	50.729161	4.623107	58.878386
H	53.132652	3.775026	60.611393
H	51.606031	4.392884	61.223283
H	52.078488	6.620051	60.132862
H	53.659987	6.005017	59.619064
H	54.214444	5.475662	62.027751
H	52.630639	6.092340	62.520842
H	54.836431	7.681393	61.367600
H	54.226948	7.731839	62.999363
H	59.760942	11.405755	65.238006
H	54.540592	11.800600	68.870550
H	50.856547	10.102721	63.916396
H	55.959712	10.750100	60.064200
H	59.606915	9.622798	67.563470
H	57.924093	9.407010	68.110908
H	59.137231	10.146388	69.197799
H	59.511296	13.281009	67.072527
H	59.582168	12.866743	68.795913
H	57.079623	11.620685	69.371765
H	52.296398	9.231515	68.644640
H	51.064813	10.320486	69.335909
H	52.777143	10.566525	69.723823
H	52.058192	13.279396	67.158456

H	52.580365	13.002211	68.835385
H	50.814691	9.745581	66.775312
H	51.211328	10.005708	61.294316
H	53.343200	10.360923	59.653484
H	58.583826	11.135395	60.415175
H	60.169604	11.414252	62.596639
H	53.040105	12.655960	62.219315
H	52.571287	12.837371	64.759869
H	52.797631	14.585517	64.608811
H	52.754214	7.672724	71.255222
H	56.192962	2.584162	65.010031
H	57.574493	8.009819	63.742776
H	53.321747	8.285170	61.629439
H	51.554581	13.541873	62.629149
H	53.027233	14.426348	62.163964
O	52.281498	7.337049	66.002815
H	53.034944	7.730954	65.479983
H	51.608424	8.038858	66.016335
O	56.483524	7.486370	67.599672
H	56.637474	7.740940	66.639926
H	57.253757	6.948588	67.848248
H	51.855049	1.324421	63.636361
Fe	54.624851	17.675886	67.226816
Fe	56.811637	15.850390	68.050493
Fe	55.216705	15.044071	65.897644
Fe	56.984533	17.135691	65.431089
S	57.490789	14.862076	66.088703
S	54.683108	17.125687	64.912577
S	56.896255	18.212354	67.531893
S	54.516738	15.435481	68.069523
C	56.384436	16.838522	71.093916
S	57.478654	15.671292	70.187027
C	53.777736	20.906312	67.046846
S	53.239997	19.342891	67.873204
C	58.430386	19.876242	64.606136
S	58.252703	18.185680	63.890146
H	55.337466	16.553125	70.943746
H	56.544032	17.854417	70.718640
H	53.148681	21.712116	67.437826
H	54.829270	21.106069	67.277263

H	58.765641	19.815020	65.646016
H	56.639674	16.782975	72.156995
H	57.469368	20.399157	64.561154
H	59.170413	20.415028	64.004823
H	53.642890	20.818753	65.963878
H	57.168829	13.084092	68.377250
H	50.537340	11.412417	66.297216

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